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Multireference Description of Nickel–Aryl Homolytic Bond Dissociation Processes in Photoredox Catalysis

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Multireference electronic structure calculations consistent with known experimental data have elucidated a novel mechanism for photo-triggered Ni(II)–C homolytic bond dissociation in Ni 2,2'-bipyridine (bpy) photoredox catalysts. Previously, a thermally assisted dissociation from the lowest energy triplet ligand field excited state was proposed and supported by density functional theory (DFT) calculations that reveal a barrier of ~30 kcal mol^{-1}. In contrast, multireference ab initio calculations suggest this process is disfavored, with barrier heights of ~70 kcal mol^{-1}, and highlight important ligand noninnocent contributions to excited state relaxation and bond dissociation processes that are not captured with DFT. In the multireference description, photo-triggered Ni(II)–C homolytic bond dissociation occurs via initial population of a singlet Ni(II)-to-bpy metal-to-ligand charge transfer (^{1}MLCT) excited state followed by intersystem crossing and aryl-to-Ni(III) charge transfer, overall a formal two-electron transfer process driven by a single photon. This results in repulsive triplet excited states from which spontaneous homolytic bond dissociation can occur, effectively competing with relaxation to the lowest energy, nondissociative triplet Ni(II) ligand field excited state. These findings guide important electronic structure considerations for the experimental and computational elucidation of the mechanisms of ground and excited state cross-coupling catalysis mediated by Ni heteroaromatic complexes.

File list (2)

Multireference Description of Nickel–Aryl Homolytic Bond Dissociation Processes in Photoredox Catalysis

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Abstract

Multireference electronic structure calculations consistent with known experimental data have elucidated a novel mechanism for photo-triggered Ni(II)–C homolytic bond dissociation in Ni 2,2'-bipyridine (bpy) photoredox catalysts. Previously, a thermally assisted dissociation from the lowest energy triplet ligand field excited state was proposed and supported by density functional theory (DFT) calculations that reveal a barrier of ~30 kcal mol^{-1}. In contrast, multireference ab initio calculations suggest this process is disfavored, with barrier heights of ~70 kcal mol^{-1}, and highlight important ligand noninnocent contributions to excited state relaxation and bond dissociation processes that are not captured with DFT. In the multireference description, photo-triggered Ni(II)–C homolytic bond dissociation occurs via initial population of a singlet Ni(II)-to-bpy metal-to-ligand charge transfer (^{1}MLCT) excited state followed by intersystem crossing and aryl-to-Ni(III) charge transfer, overall a formal two-electron transfer process driven by a single photon. This results in repulsive triplet excited states from which spontaneous homolytic bond dissociation can occur, effectively competing with relaxation to the lowest energy, nondissociative triplet Ni(II) ligand field excited state. These findings guide important electronic structure considerations for the experimental and computational elucidation of the mechanisms of ground and excited state cross-coupling catalysis mediated by Ni heteroaromatic complexes.

Introduction

Merging thermal catalysis with photochemistry (i.e., photoredox catalysis) has provided new, more sustainable routes to bond activations and coupling reactions in organic synthesis.[1–10] An extension of solar energy conversion, photoredox catalysis utilizes photosensitizers to harvest photon energy and transform it into chemical potential to drive single electron transfer (SET) processes to generate reactive high- and/or low-valent species and important organic radicals. However, photoredox reactions feature complex mechanisms that are challenging to elucidate, and our understanding of how photon energy drives organic transformations is therefore still growing.

Beyond SET, photosensitized energy transfer can form photocatalyst excited states that can be uniquely reactive relative to ground states.[11–16] The photocatalyst can also potentially act as both the light-absorbing and catalytic unit through direct excitation.[17,18] In direct excitation and energy transfer mediated catalysis, the ultrafast photophysical processes of transition metal excited state relaxation can also contribute to reactivity.[9] Notably, Ni(II) complexes of 2,2'-bipyridine (bpy) exhibit photocatalytic activity for coupling reactions using either energy transfer[11,19] or direct excitation.[20] Several mechanistic hypotheses have been discussed and are summarized in Figure 1. In one scenario, energy transfer to a Ni(II)-bpy aryl acetate complex induces reductive elimination from a triplet excited state of Ni(II) (Figure 1A, bottom), originally proposed to be ligand field in nature.[11] Ni(II)-to-bpy metal-to-ligand charge transfer (MLCT) excited states have also been suggested to: 1) mediate bimolecular electron transfer to generate Ni(I) and Ni(III) species for catalysis,[17] or 2) directly mediate reductive elimination.[21] The latter consideration encompasses the one-electron oxidatively induced ground state formal Ni(III) reactivity discovered by Hillhouse and co-workers.[22,23]

Thermally assisted homolytic Ni(II)–C bond dissociation from photochemically formed triplet ligand field excited states in Ni(II)-bpy aryl halide complexes has also been proposed.[18] This process results in the formation of formal Ni(I) and aryl radicals (Figure 1A, top). While it is unclear whether these species initiate a subsequent Ni(I)/Ni(III) catalytic cycle, this represents an intriguing means to photochemically generate reduced Ni species and organic radicals for ground state thermal catalysis.[18,20] Overall, more detailed experimental and theoretical descriptions of the ground state bonding and excited state relaxation processes in Ni-bpy complexes (and other Ni heteroaromatic complexes[24]) are critical for developing synthetic applications.

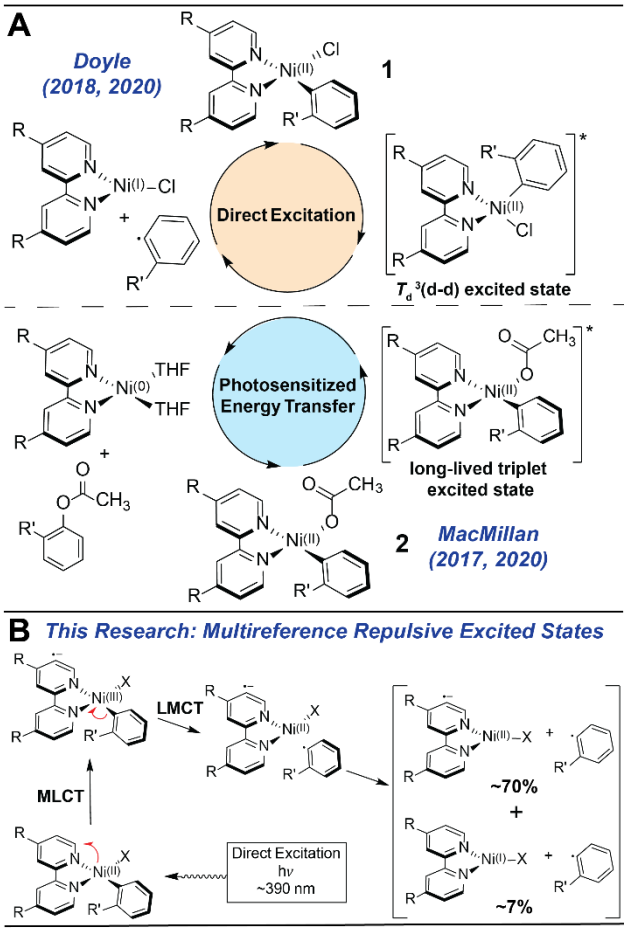

Figure 1. (A) Two previous mechanistic hypotheses related to Ni-bpy photoredox catalysis and (B) findings in this study.

Here we describe a new electronic structural framework to interpret experimental data on Ni(II)-bpy complexes of relevance to photoredox catalysis. Of particular importance is the multireference description (relative to density functional theory (DFT)), which manifests in mixed ground and excited state wave functions and potential energy surfaces (PESs) in Ni(II)–C homolytic bond dissociation. Intractable barriers are found for thermal bond dissociation from the lowest energy triplet ligand field excited state within the multireference framework. However, higher energy repulsive triplet excited states are found here and are proposed to be responsible for homolytic bond dissociation. These triplet excited states feature a high-spin Ni(II) coupled to anionic bpy and neutral aryl radicals and can be generated from initial ^{1}MLCT excitation (Ni(II)-to-bpy) followed by intersystem crossing and intramolecular charge transfer (aryl-to-Ni(III)) (Figure 1B).

Computational Methods

Calculations were performed using ORCA[25,26] version 4.2.1. The BP86[27-29] functional was used for geometry optimizations and frequency calculations, including both full geometry optimizations and constrained optimizations where the Ni–C bond length was systematically varied. The 6-311G(d)[30] basis set was used on all atoms, and AutoAux[31] was used as the auxiliary basis set. Split-RI-J, the default and recommended version of resolution of identities[32–35] (RI) approximation was used. The finest available DFT grids were used (GRID7 NOFINALGRID). Very tight SCF convergence criteria, which has a convergence tolerance of 10^{-9} Hartrees, was applied for all DFT calculations. The restricted Kohn-Sham formalism (RKS) was used for the singlet ground state optimizations; the unrestricted Kohn-Sham formalism (UKS) was used for the triplet optimizations. Additional single point calculations using the B3LYP[28,36] functional, the def2-TZVP[37] basis, and implicit solvation by tetrahydrofuran (THF) modeled by the conductor-like polarized continuum model[38] (CPCM) were performed on optimized structures. Here the RIJCOSX[39] approximation was used with fine DFT grids (GRID7 NOFINALGRID GRIDX9). At this level of theory, broken-symmetry singlet (BSS) and unrestricted triplet single point calculations were performed on the S=0 and S=1 optimized geometries, respectively. Likewise, TDDFT calculations were performed using these same settings. Applying a Yamaguchi spin correction[40,41] did not significantly affect the BSS dissociations energies of **1** and **2**. It lowered the dissociation energy of **1** from 43.3 kcal mol^{-1} to 41.7 kcal mol^{-1} (Table S1P); it barely changed the dissociation energy of **2** from 44.9 kcal mol^{-1} to 45.1 kcal mol^{-1} (Table S2L). Sample input DFT and TDDFT parameters are given on page S3.

Quasidegenerate N-electron valence state second-order perturbation theory[42] (QD-NEVPT2) corrected complete active space self-consistent field (CASSCF) single point calculations were performed on DFT optimized geometries. Tight SCF convergence criteria with an energy tolerance of 10^{-7} Hartrees were applied. The def2-TZVP basis set was used on all atoms, and the RIJCOSX approximation was employed. Note that the number of states averaged was varied (see Tables S1G-1 – S1G-3), and it was found that a state-averaging with fifteen singlets and twenty-five triplets yielded a thorough description of the ground and excited states of interest while maintaining reasonable computational costs. Therefore, state-averaged CASSCF/QD-NEVPT2 single point calculations utilized fifteen singlets and twenty-five triplets throughout. The recommended Nakano formalism was used, and the corresponding CI-vectors are tabulated below.

A comparison between gas phase and solvent corrected CASSCF/QD-NEVPT2 single point calculations yielded qualitatively similar results at both the singlet equilibrium geometry and at longer Ni–C distances (3.2 Å for **1** and 3.1 Å for **2**); therefore, gas phase calculations were conducted on all structures (comparisons are tabulated in the Supporting Information). Sample input files for CASSCF/QD-NEVPT2 calculations are given on page S3.

The size of the active space was varied until a thorough description of **1** and **2** was reached (comparisons between active space sizes are tabulated in the Supporting Information). Active spaces are shown in Figures S1C and S1E for **1** (S=0 and S=1) and Figure S2C and S2E for **2** (S=0 and S=1). The first 10-20 lowest energy roots, CI vectors, transitions, and oscillator strengths are tabulated in the Supporting Information. An active space consisting of nine orbitals filled with ten electrons (9o/10e): d(xy), d(z^2), d(xz), d(yz), a pair of bonding and antibonding orbitals from the d(x^2-y^2) and the C(sp^2) orbital on the dissociating phenyl group, and three π* orbitals on the bipyridine ligand, were found to be thorough descriptors of the S=0 equilibrium geometry of **1**, while an additional orbital was added for **2**. The additional orbital in **2** is a bonding d(xy)/C(π) orbital (see Figure S2C), which was kept in the active space due to its partially unfilled occupancy of 1.93 (for compound **1**, this orbital has occupancy of ~2 (1.99), and thus was not needed to generate a complete active space). However, as can be seen in Table S2C1-3, the additional orbital in **2** was not involved in any critical transitions. At all other Ni–C bond lengths, the third bpy π* orbital exhibited very low occupancy and was removed to aid convergence. For example, the ten electrons in nine orbitals CASSCF calculation using the 3.6 Å geometry of **1**, the third π* orbital had an extremely low active space occupancy value of 0.00004.

As the Ni–C bond was elongated and eventually cleaved, the molecular geometry along the singlet surface approached that of the optimized triplet surface. This observation is particularly clear for **2**. Geometry coordinates along the Ni–C scan are listed in the Appendix portion of the Supporting Information. The active space for the triplet scan of **1** again consisted of the ten electrons in eight orbitals (active space with the third π* removed, Figure S1E). Here the third bpy π* again had very low active space occupancy values (~0.0001). This was true in geometries ranging from 2.0 Å to 3.6 Å. For triplet structures of **1** with a short Ni–C bond (between 1.6-2.0 Å), the second π* orbital was similarly removed to aid convergence. For the triplet scan of **2**, it was possible to use an active space of ten electrons in nine orbitals active space for the entire scan (Figure S2E).

Results and Discussion

Homolytic bond dissociation is an inherently multireference process that can pose difficulties for DFT.[43,44] Analyses therefore began by comparing the ground state wave functions of Ni(II)($^{t\text{-}Bu}$bpy)(*o*-tolyl)Cl (**1**) and Ni(II)(bpy)(ph)(ac) (ph = phenyl, ac = acetate) (**2**), as well as their lowest energy singlet and triplet bond dissociation energies (BDEs) using both DFT and multireference ab initio calculations (i.e., CASSCF/QD-NEVPT2[42]) within ORCA.[25,26]

CASSCF/QD-NEVPT2 calculations on **1** and **2** exhibit appreciable ground state multireference character (Figures S1C/S2C and Tables S1C/S2C-1). Using a nine orbital, ten electron active space (Figure S1C), the dominant contributions to the configuration interaction (CI) vector of the singlet ground state of **1** are ~58 % low-spin d^8 (closed shell singlet, CSS) and ~22 % ^{1}MLCT (Table S1E). Similar values are obtained for **2** (~57% CSS and ~23 % ^{1}MLCT) (Table S2D-2). With only an eight electron, five 3d-orbital active space, the low-spin d^8 character increases to ~95 % in both **1** and **2** (Table S1A-2/S2B-2). Thus, the unoccupied bpy π* orbitals, which have high active space occupancies, play a critical role in the degree of multireference ground state bonding.

It is interesting to consider the multireference data in the context of the DFT bonding description. The low-spin $d(x^2\text{-}y^2)$ ground states of **1** and **2** are highly covalent (~56/57 % Ni(II) and ~11/13 % bpy character), with some back-bonding (~7-8 % occupied Ni(II) character in the bpy-based unoccupied π* orbitals of both **1** and **2**) (Figure S1B/S2B). This highly covalent bonding framework is not particularly amenable to formal redox state assignment and is more consistent with a multireference bonding description.[45,46]

PESs for Ni(II)–C bond dissociations from **1** and **2** are given in Figures 2A and S2G, respectively. The DFT BDEs are ~43 kcal mol^{-1} and ~31 kcal mol^{-1} starting from the relaxed, lowest energy singlet and triplet structures of **1**, respectively, consistent with the ~32 kcal mol^{-1} from a study invoking thermal homolysis on the triplet PES.[18] Values for **2** are similar (~45 kcal mol^{-1} and ~38 kcal mol^{-1}). The multireference bond dissociation is fundamentally different than DFT, with significantly higher BDEs (~87/65 kcal mol^{-1} and 73/70 kcal mol^{-1} from the lowest energy singlet and triplet states of **1**/**2**), suggesting the Ni(II)–C bonds are stronger than in DFT and will not be thermally cleaved, even upon formation of the relaxed lowest energy triplet ligand

field excited state. This difference is important, as the ~30 kcal mol^{-1} barrier was used to rationalize photochemical formation of radicals and reduced Ni species from **1**.[18]

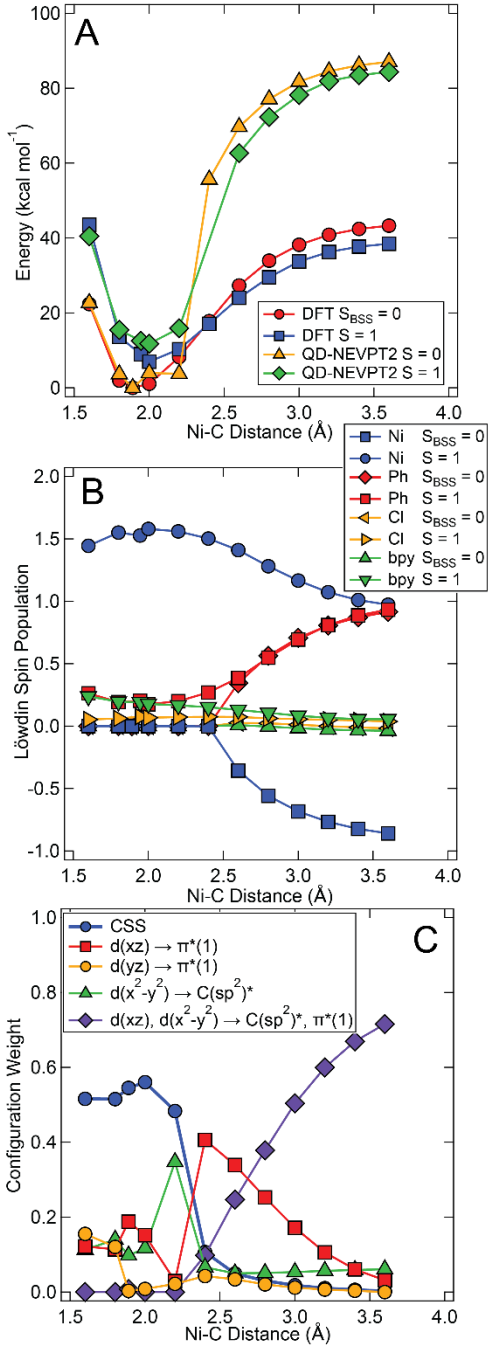

Figure 2. Ni(II)–C bond dissociation from the lowest energy singlet and triplet states in **1**. (A) Relaxed DFT vs CASSCF/QD-NEVPT2 PESs and (B) DFT Löwdin spin densities for both the singlet (BSS) and triplet states and (C) the CASSCF/QD-NEVPT2 lowest energy singlet CI vector.

From Löwdin spin density plots in Figures 2B and S2H, the DFT-based homolytic bond dissociation results in the formation of Ni(I) and neutral aryl radicals for **1** and **2**. The compositions of the multireference ground state CI vectors of **1** and **2** upon bond dissociation from the singlet ground state are given in Figures 2C and S2I, respectively, and describe the nature of bond homolysis. Upon initial elongation of the Ni–C bond, the amount of low-spin d^8 character (CSS) decreases significantly, with a concomitant increase in the weighting of ^{1}MLCT character at 2.4 Å, beyond which the CI vector becomes dominantly $d(xz)/d(x^2\text{-}y^2) \rightarrow C(sp^2)^*/\pi^*$, formally corresponding to a high-spin Ni(II) coupled to anionic bpy and neutral aryl radicals. Some additional formal Ni(I) character is also present (~7 %). Independent DFT vs multireference calculations on the formal Ni(I) species after homolytic bond dissociation (Figure 3) further support this description. Notably, similar ligand redox has been observed for reduced formal Ni(I) species in ground state cross-coupling reactions.[24,47]

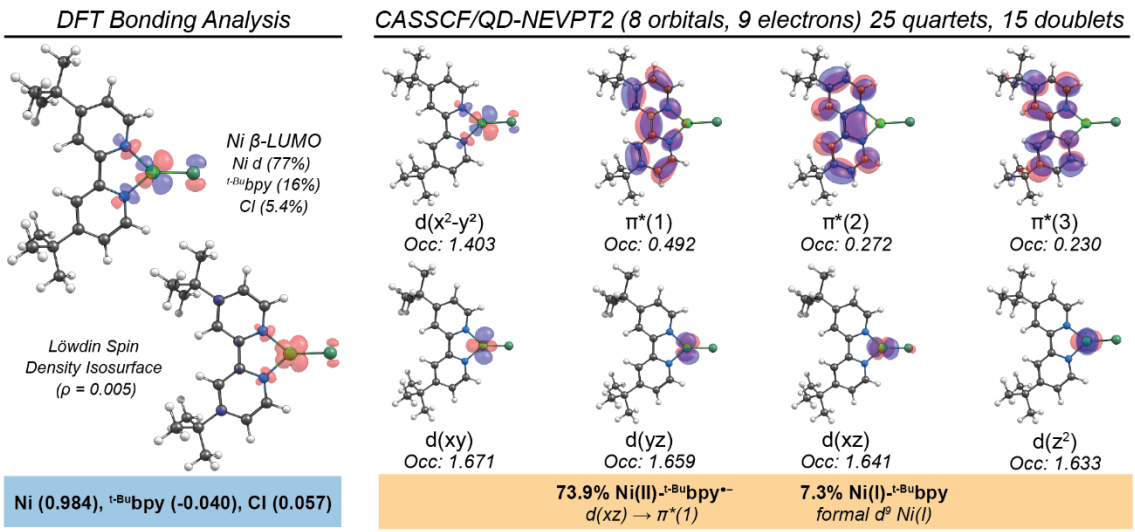

Figure 3. DFT (left) vs CASSCF/QD-NEVPT2 (right) description of the formal Ni(I) species formed upon homolytic Ni–C bond cleavage.

Given the intractability of thermally assisted Ni(II)–C homolysis and radical formation from the lowest energy triplet ligand field excited states, we now further describe the excited state PESs/manifolds of **1** and **2** to develop new understanding of the mechanism of homolytic bond dissociation. TDDFT and CASSCF/QD-NEVPT2 calculated excited state manifolds at the ground state singlet relaxed structures of **1** and **2** are given in Figure S1G and Tables S1I-K, S2A, and

S2C. Both methods predict a set of lower and higher energy ^{1,3}MLCTs. However, their relative oscillator strengths differ somewhat from one another and, for **1**, the experimental spectrum.

The CASSCF/QD-NEVPT2 ground and excited state PESs along the Ni(II)–C coordinate of **1** and **2** are given in Figure 4 and S2J, respectively, while the analogous TDDFT PESs are given in Figure S1F and S2K, respectively. From Figure 4, repulsive excited states are present (black, red, and yellow lines). The higher energy MLCT excited states (**A** in Figure 4) cross the repulsive surfaces at Ni–C bond distances of ~2.3–2.4 Å (circled in Figure 4) in both **1** and **2** with an activation energy from the Franck-Condon point of ~25 kcal mol^{-1}. Thus, the multireference approach predicts homolytic bond dissociation occurs via population of a ^{1}MLCT excited state (Ni(II)-to-bpy) followed by an intersystem crossing and intramolecular charge transfer (aryl-to-Ni(III)) (Figure 1B). The intersystem crossing could occur between the ^{1,3}MLCT states or the ^{1}MLCT and dissociative triplet state. Overall, this represents a novel homolytic bond dissociation mechanism, which we propose derives from the redox noninnocent and multireference ground and excited state bonding in Ni(II)-bpy complexes.

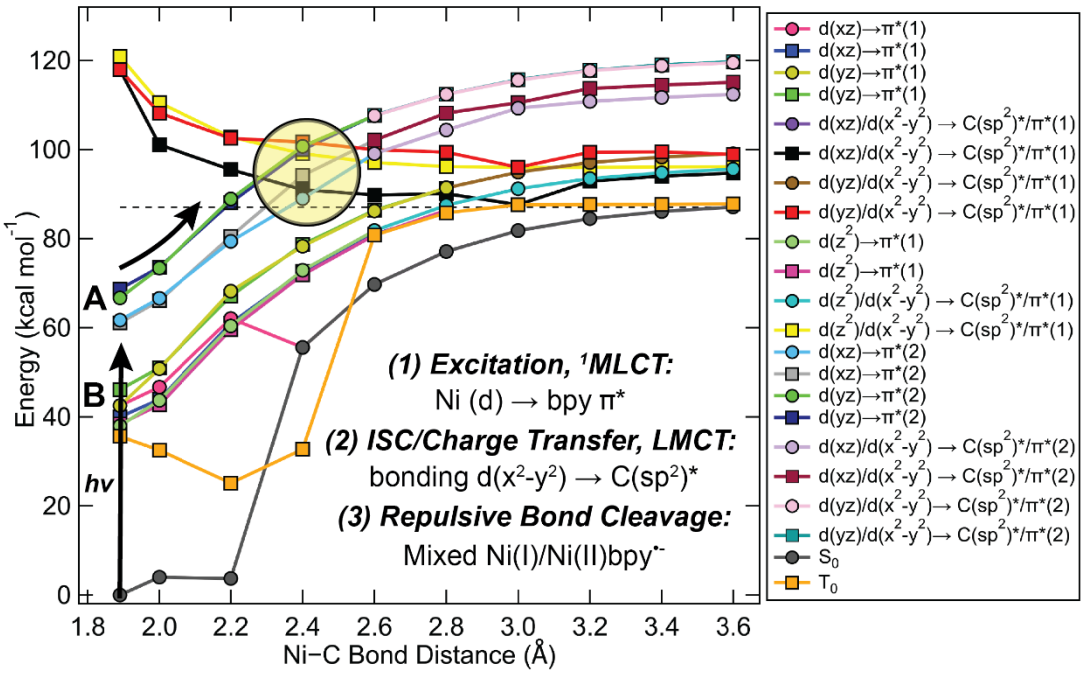

Figure 4. CASSCF/QD-NEVPT2 relaxed ground and excited state PESs along the Ni–C coordinate of **1**. Vertical excitation (black vertical arrow), the higher (A) and lower energy (B) manifolds of MLCTs, and the crossings between the higher energy MLCTs and repulsive triplets (circled) are depicted. Singlet states, circles; triplets, squares.

Experimentally, the lowest energy triplet ligand field excited states of Ni(II)-bpy aryl halide complexes are populated in ~5-10 ps.[18] Given an estimated Ni(II)–C frequency of ~250 cm^{-1}, ~40-80 vibrational periods could occur to drive intersystem and surface crossings that could compete with population of the lowest energy triplet ligand field state. A higher energy aryl vibration (~650 cm^{-1}; Figures S1I/S2L for **1** and **2**, respectively) exhibiting significant changes in Ni–C bond distance may also provide ~100-200 vibrational periods to drive these processes.

The yield of cross-coupled product obtained from direct excitation of **1** is incident light dependent; high yields are only observed with UV light (390-395 nm or ~70 kcal mol^{-1}),[20] corresponding to excitation into the higher energy manifold of MLCT states (Figure 4). Of particular relevance to compound **2**, variations in the energy of the photosensitizer triplet state demonstrated C–O coupling occurs when ~40-45 kcal mol^{-1} is transferred to the Ni catalyst.[11] This energy would excite complexes to the lower energy manifold of MLCT states (Figure 4, S2J), resulting in thermodynamically unfavorable radical formation (~45 kcal mol^{-1}) for both **1** and **2**. Thus, an alternative relaxation pathway and mechanism may exist for photosensitized cross-coupling. In fact, triplet ligand field excited state formation, reductive elimination, and homolytic bond dissociation may all be possible for a given Ni(II)-bpy complex. We believe the ligands in addition to bpy will be of particular importance in determining the relative propensity for specific relaxation pathways. For example, reductive elimination is disfavored for the aryl halide (**1**) relative to the aryl carboxylate (**2**). This may preferentially lead to excited state processes that favor the formation of radicals and ligand field excited states over an intractable photosensitized or direct excitation induced reductive elimination. A future study will aim to elucidate and analyze these potentially competitive pathways.

Conclusions

In summary, we have provided a new electronic structural framework to interpret UV light-induced homolytic bond dissociation in Ni(II)-bpy complexes of relevance for photoredox catalysis. Compared to DFT, multireference ab initio calculations predict: 1) thermal homolysis from the lowest energy triplet ligand field excited state is not energetically favorable (barriers: DFT ~30 kcal mol^{-1}, CASSCF/QD-NEVPT2 ~70 kcal mol^{-1}), 2) initial population of a Ni(II)-to-bpy ^{1}MLCT excited state can be followed by intersystem crossing and aryl-to-Ni(III) intramolecular charge transfer, resulting in the formation of repulsive triplet excited states

described as a high-spin Ni(II) coupled to anionic bpy and neutral aryl radicals. Formally, this represents an overall two-electron transfer process driven by a single photon. The formation of repulsive excited states likely also competes with relaxation to the experimentally observed triplet ligand field excited state, which further relaxes to the ground state without radical formation. 3) The immediate products of homolytic bond dissociation are not Ni(I)-bpy and an aryl radical as described by DFT, but rather, from the multireference CI vector, a dominantly high-spin Ni(II) coupled to a redox active bpy anion radical ligand, similar to descriptions for formal Ni(I) intermediates in ground state thermal cross-coupling catalysis.[24,47]

Supporting Information

Details of computational methods; tabulation of TDDFT and CASSCF/QD-NEVPT2 energetics; tabulation of CASSCF/QD-NEVPT2 CI-vectors; plotted data for **2** analogous to data for **1** presented in manuscript; DFT optimized structures.

Acknowledgments

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Supporting Information

Multireference Description of Nickel–Aryl Homolytic Bond Dissociation Processes in Photoredox Catalysis

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A. Example Input Files

A.1. Example DFT Input

```
! RKS BP86 6-311G(d) AutoAux
! TIGHTOPT FREQ
! RI VeryTightSCF GRID7 NOFINALGRID
! SlowConv PrintBasis LargePrint

%pal nprocs 16
end
%maxcore 9000

%method
  Z_solver DIIS
  Z_shift 0.5
end

*xyzfile 0 1 File.xyz
```

A.2. Example TDDFT Input

```
! UKS B3LYP def2-tzvp AutoAux SP RIJCOSX
! VeryTightSCF GRID7 NOFINALGRID GRIDX9
! SlowConv PrintBasis LargePrint CPCM(THF)
! MORead
%moinp "File.gbw"

%pal nprocs 16
end
%maxcore 9000

%tddft
  nroots 50
  maxdim 5
end

*xyzfile 0 3 File.xyz
```

A.3. Example CASSCF/QD-NEVPT2 Input

```
! def2-TZVP AutoAux RIJCOSX TightSCF CPCM(THF)
! LargePrint MOREAD
%moinp "File.gbw"

%casscf
  norb    9
  nel     10
  mult    3,1
  nroots 25,15
  TrafoStep RI
  MaxIter 400
  etol 1e-7
  printwf det
  orbstep SuperCI
  switchstep DIIS
  ShiftUp 2.0
  ShiftDn 2.0
  ptmethod sc_nevpt2
  ptsettings
  qdtype qd_vanvleck
  end
rel
  dosoc true
  gtensor true
  dtensor true
  end
end

%pal
  nprocs 16
end
%maxcore 9000

* xyzfile 0 1 File.xyz
```

B. Tables Part 1: Compound *1*

Table S1A-1. Compound **1** – CASSCF/QD-NEVPT2 lowest transition energies in the gas phase (5o, 8e Active Space) – 10 triplet roots, 10 singlet roots. Active Space Orbitals (in order for CI vector notation below): d(z^2), d(xz), d(yz), d(xy), d(x^2-y^2).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
0	0	1	---	---	22220	---	0.95128
					02222	---	0.02052
1	0	3	1090.8	26.2	12221	---	0.99927
					---	---	---
2	1	3	1009.0	28.3	21221	---	0.75971
					22121	---	0.21841
3	2	3	884.4	32.3	22121	---	0.75325
					21221	---	0.21711
4	3	3	614.5	46.5	22211	---	0.93594
					21122	---	0.06344
5	1	1	420.1	68.1	21221	0.0000024	0.77158
					22122	---	0.20180
6	2	1	414.9	68.9	12221	0.0000399	0.97842
					22022	---	0.00639
7	3	1	395.1	72.4	22121	0.0001334	0.77021
					21221	---	0.20266
8	4	1	382.6	74.7	22211	0.0001352	0.99872
					---	---	---
9	4	3	292.0	97.9	21212	---	0.45857
					22112	---	0.37735
10	5	3	288.9	98.9	12212	---	0.99393
					21122	---	0.00338

Table S1A-2. Compound **1** – CASSCF/QD-NEVPT2 lowest transition energies with CPCM(THF) (5o, 8e Active Space) – 10 triplet roots, 10 singlet roots. Active Space Orbitals (in order for CI vector notation below): d(z^2), d(xz), d(yz), d(xy), d(x^2-y^2).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
0	0	1	---	---	22220	---	0.94984
					02222	---	0.02128
1	0	3	1224.5	23.4	12221	---	0.99185
					---	---	---
2	1	3	1089.4	26.2	21221	---	0.94767
					22121	---	0.03109
3	2	3	973.7	29.4	22121	---	0.93700
					21221	---	0.03119
4	3	3	633.7	45.1	22211	---	0.92979
					21122	---	0.06922
5	1	1	431.4	66.3	21221	0.0000031	0.86047
					12221		0.09338
6	2	1	431.3	66.3	12221	0.0000287	0.88620
					20222		0.00722
7	3	1	410.5	69.6	22121	0.0001197	0.94493
					21221		0.02702
8	4	1	387.8	73.7	22211	0.0001278	0.99747
					---		---
9	4	3	301.8	94.8	21212	---	0.59108
					22112	---	0.23535
10	5	3	299.7	95.4	12212	---	0.99260
					21122	---	0.00415

Table S1B. Compound **1** – CASSCF/QD-NEVPT2 lowest transition energies in the gas phase. 9o, 10e Active Space – 25 triplet roots, 15 singlet roots. Orbitals (in order for CI vector notation below): d(xy), d(x^2-y^2)/C(sp^2), d(yz), d(z^2), d(xz), d(x^2-y^2)/C(sp^2)*, π*(1), π*(2), π*(3).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
0	0	1	---	---	222220000	---	0.5455
					222210100	---	0.1876
					212221000	---	0.0977
1	0	3	802.3	35.6	222121000	---	0.4035
					222210100	---	0.1917
2	1	3	774.8	36.9	222120100	---	0.6406
					222210100	---	0.1186
3	1	1	752.5	38.0	222120100	0.0006862	0.8166
					202122100	---	0.0850
4	2	3	733.8	39.0	221221000	---	0.2244
					222210100	---	0.2117
5	3	3	715.5	40.0	221221000	---	0.2533
					222210100	---	0.2197
6	2	1	672.0	42.5	221220100	0.0649528	0.4507
					222210100	---	0.2848
7	4	3	668.3	42.8	222211000	---	0.4913
					221221000	---	0.2821
8	5	3	620.8	46.1	221220100	---	0.7066
					222210100	---	0.0871
9	3	1	604.1	47.3	221220100	0.1224866	0.3511
					222210100	---	0.2756
10	6	3	551.6	51.8	122221000	---	0.6719
					221212000	---	0.0803
11	7	3	480.7	59.5	222120010	---	0.7737
					202122010	---	0.0829
12	4	1	479.5	59.6	222120010	0.0003566	0.7222
					202122010	---	0.0773
13	5	1	472.4	60.5	122220100	0.0001327	0.7056
					221211100	---	0.0791
14	8	3	468.1	61.1	222210010	---	0.7214
					221220010	---	0.0877
15	6	1	463.2	61.7	222210010	0.0858212	0.3931
					221220010	---	0.2037
16	9	3	463.0	61.8	122220100	---	0.7507
					221211100	---	0.0792
17	7	1	439.3	65.1	222120001	0.0000514	0.7108
					202122001	---	0.0744
18	8	1	428.4	66.7	221220010	0.0799110	0.3735
					222210001	---	0.3188
19	10	3	424.0	67.4	222120001	---	0.7783
					202122001	---	0.0812
20	11	3	416.1	68.7	221220010	---	0.6613
					222210010	---	0.0772

Table S1C. Compound **1** – CASSCF/QD-NEVPT2 Lowest transition energies with CPCM(THF) 9o, 10e Active Space – 25 triplet roots, 15 singlet roots. Orbital (in order for CI vector notation below): d(xy), bonding d(x^2-y^2)/C(sp^2), d(yz), d(xz), d(z^2), d(x^2-y^2)/C(sp^2)*, π*(1), π*(2), π*(3).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
0	0	1	---	---	222220000	---	0.5752
					222120100	---	0.1521
					212221000	---	0.1097
1	0	3	832.8	34.3	222211000	---	0.7672
					212212000	---	0.1435
2	1	3	758.1	37.7	222121000	---	0.4011
					221221000	---	0.3532
3	2	3	712.3	40.1	222210100	---	0.3289
					221221000	---	0.3246
4	3	3	678.4	42.2	222210100	---	0.4433
					222121000	---	0.2503
5	1	1	671.4	42.6	222210100	0.0008408	0.8161
					202212100	---	0.0876
6	4	3	647.1	44.2	222120100	---	0.7582
					202122100	---	0.0850
7	2	1	604.2	47.3	221220100	0.0622469	0.4193
					222120100	---	0.3382
8	5	3	574.3	49.8	221220100	---	0.5752
					122221000	---	0.1682
9	6	3	551.4	51.9	122221000	---	0.5491
					221220100	---	0.1783
10	3	1	546.6	52.3	221220100	0.1520657	0.3722
					222120100	---	0.2674
11	4	1	444.6	64.3	222120010	0.1043472	0.5270
					221220010	---	0.1267
12	7	3	441.9	64.7	222210010	---	0.7193
					222210001	---	0.0917
13	5	1	440.4	64.9	122220100	0.0001963	0.4135
					222210010	---	0.3424
14	6	1	437.3	65.4	222210010	0.0003333	0.4320
					122220100	---	0.3239
15	8	3	424.8	67.3	222120010	---	0.7541
					202122010	---	0.0870
16	9	3	423.2	67.5	122220100	---	0.7670
					221121100	---	0.0820
17	10	3	410.6	69.6	222210001	---	0.7193
					222210010	---	0.0922
18	7	1	407.1	70.2	222121000	0.0002537	0.6733
					221221000	---	0.1149
19	8	1	401.3	71.3	222211000	0.0305023	0.2808
					221220010	---	0.2155
20	9	1	399.9	71.5	122221000	0.0329884	0.4648
					222211000	---	0.1385

Table S1D. Compound **1** – CASSCF/QD-NEVPT2 composition of the singlet equilibrium ground state in gas phase. 9o, 10e Active Space – 25 triplet roots, 15 singlet roots. Orbitals: bonding $d(x^2\text{-}y^2)/C(sp^2)$, d(xy), d(xz), d(yz), $d(z^2)$, $d(x^2\text{-}y^2)/C(sp^2)^*$, π*(1), π*(2), π*(3).

CI Vector	Transition	Contribution
222220000	Closed shell singlet (CSS) d^8	0.5455
222210100	d(xz) → π*(1)	0.1876
212221000	bonding $d(x^2\text{-}y^2)/C(sp^2)$ → $d(x^2\text{-}y^2)/C(sp^2)^*$	0.0977
221220001	d(yz) → π*(3)	0.0400
222210010	d(xz) → π*(2)	0.0312
202212100	2x[bonding $d(x^2\text{-}y^2)/C(sp^2)$] + d(xz) → 2x[$d(x^2\text{-}y^2)/C(sp^2)^*$] + π*(1)	0.0224
222121000	$d(z^2)$ → $d(x^2\text{-}y^2)$]	0.0090
212211100	bonding $d(x^2\text{-}y^2)/C(sp^2)$ + d(xz) → $d(x^2\text{-}y^2)/C(sp^2)^*$ + π*(1)	0.0083
222022000	2x[$d(z^2)$] → 2x[$d(x^2\text{-}y^2)/C(sp^2)^*$]	0.0079
220222000	2x[d(yz)] → 2x[$d(x^2\text{-}y^2)/C(sp^2)^*$]	0.0056
222202000	2x[d(xz)] → 2x[$d(x^2\text{-}y^2)/C(sp^2)^*$]	0.0055
201222001	2x[bonding $d(x^2\text{-}y^2)/C(sp^2)$] + d(yz) → $d(x^2\text{-}y^2)/C(sp^2)^*$ + π*(3)	0.0042
202212010	2x[bonding $d(x^2\text{-}y^2)/C(sp^2)$] + d(xz) → $d(x^2\text{-}y^2)/C(sp^2)^*$ + π*(2)	0.0040
122221000	d(xz) → $d(x^2\text{-}y^2)/C(sp^2)^*$	0.0029
221220100	d(yz) → π*(1)	0.0029
Sum of CSS		**55%**
Sum of all MLCT		**26%**
Sum of all d-d		**13%**
Sum of mixed MLCT + d-d		**3.9%**

Table S1E. Compound **1** – CASSCF/QD-NEVPT2 composition of the singlet equilibrium ground state with CPCM(THF). 9o, 10e Active Space – 25 triplet roots, 15 singlet roots. Orbitals: bonding $d(x^2\text{-}y^2)/C(sp^2)$, d(xy), d(xz), d(yz), $d(z^2)$, $d(x^2\text{-}y^2)/C(sp^2)^*$, π*(1), π*(2), π*(3).

CI Vector	Transition	Contribution
222220000	Closed shell singlet (CSS) d^8	0.5752
222120100	d(xz) → π*(1)	0.1521
212221000	bonding $d(x^2\text{-}y^2)/C(sp^2)$ → $d(x^2\text{-}y^2)/C(sp^2)^*$	0.1097
221220001	d(yz) → π*(3)	0.0383
222120010	d(xz) → π*(2)	0.0256
202122100	2x[bonding $d(x^2\text{-}y^2)/C(sp^2)$] + d(xz) → 2x[$d(x^2\text{-}y^2)/C(sp^2)^*$] + π*(1)	0.0192
222211000	$d(z^2)$ → $d(x^2\text{-}y^2)/C(sp^2)$	0.0101
221220100	d(yz) → π*(1)	0.0090
222202000	2x[$d(z^2)$] → 2x[$d(x^2\text{-}y^2)/C(sp^2)^*$]	0.0090
212121100	bonding $d(x^2\text{-}y^2)/C(sp^2)$ + d(xz) → $d(x^2\text{-}y^2)/C(sp^2)^*$ + π*(1)	0.0073
220222000	2x[d(yz)] → 2x[$d(x^2\text{-}y^2)/C(sp^2)^*$]	0.0063
222022000	2x[d(xz)] → 2x[$d(x^2\text{-}y^2)/C(sp^2)^*$]	0.0063
201222001	2x[bonding $d(x^2\text{-}y^2)/C(sp^2)$] + d(yz) → 2x[$d(x^2\text{-}y^2)/C(sp^2)^*$] + π*(3)	0.0041
202122010	2x[bonding $d(x^2\text{-}y^2)/C(sp^2)$] + d(xz) → 2x[$d(x^2\text{-}y^2)/C(sp^2)^*$] + π*(2)	0.0034
Sum of CSS		**58%**
Sum of all MLCT		**22%**
Sum of all d-d		**14%**
Sum of mixed MLCT + d-d		**3.4%**

Table S1F. Compound **1** with Ni–C distance of 3.20 Å – CASSCF/QD-NEVPT2 lowest transition energies in gas phase. 8o,10e Active Space – 25 triplet roots, 15 singlet roots. Orbitals: d(xy), d(yz), $d(z^2)$, d(xz), bonding $d(x^2\text{-}y^2)/C(sp^2)$, $d(x^2\text{-}y^2)/C(sp^2)$*, π*(1), π*(2).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
0	0	3	---	---	22211110	---	0.5998
					22212010	---	0.1057
					22221100	---	0.0567
1	0	3	9086.0	3.1	22211110	---	0.7446
					22112110	---	0.0600
2	1	3	3630.2	7.9	22121110	---	0.8144
					22122010	---	0.1216
3	2	3	3417.1	8.4	22211110	---	0.7561
					22212010	---	0.0919
4	1	1	3189.5	9.0	22121110	0.0000059	0.8124
					22122010	---	0.1225
5	3	3	2489.9	11.5	22121110	---	0.9789
					12221110	---	0.0509
6	4	3	2304.7	12.4	21221110	---	0.7601
					21222010	---	0.1103
7	2	1	2285.4	12.5	21221110	0.0000005	0.6956
					21222010	---	0.1058
8	5	3	1919.3	14.9	21221110	---	0.8607
					22211110	---	0.0484
9	6	3	1172.8	24.4	22220110	---	0.7851
					22221010	---	0.0762
10	3	1	1170.0	24.4	22220110	0.0000682	0.7229
					22221010	---	0.0724
11	4	1	1097.4	26.1	22211101	0.0222545	0.2581
					12221110	---	0.2436
12	5	1	1090.0	26.2	22211101	0.0361406	0.4130
					21212110	---	0.1455
13	7	3	1061.0	27.0	12221110	---	0.4604
					21212110	---	0.4285
14	8	3	1030.4	27.7	22211101	---	0.7389
					22212001	---	0.0804
15	9	3	1003.5	28.5	12221110	---	0.4832
					21212110	---	0.4057
16	10	3	994.6	28.8	22121101	---	0.8005
					22122001	---	0.1199
17	6	1	993.3	28.8	22121101	0.0000753	0.8085
					22122001	---	0.1212
18	11	3	979.4	29.2	22211101	---	0.8202
					22112101	---	0.0673
19	12	3	911.0	31.4	22121101	---	0.9880
					12221101	---	0.0051
20	7	1	863.0	33.1	21221101	0.0022399	0.7256
					21222001	---	0.1076

Table S1G-1. Compound **1** – CASSCF/QD-NEVPT2 composition of the singlet equilibrium ground state while varying number of singlet roots. 9o, 10e Active Space – 25 triplet roots, *X* singlet roots (where *X* ranged from 15 to 40). Orbitals: bonding $d(x^2-y^2)/C(sp^2)$, d(xy), d(xz), d(yz), $d(z^2)$, $d(x^2-y^2)/C(sp^2)^*$, π*(1), π*(2), π*(3).

Weights of Three Most Dominant Terms in CI-Vector (# Triplets / # Singlets)							
Configuration	**25/15 CPCM**	**25/15 Gas**	**25/20 Gas**	**25/25 Gas**	**25/30 Gas**	**25/35 Gas**	**25/40 Gas**
CSS	0.5752	0.5455	0.5346	0.5202	0.5029	0.4853	0.4733
d(xz) → π*(1)	0.1521	0.1876	0.1149	0.1321	0.1224	0.1316	0.1198
bonding $d(x^2-y^2)/C(sp^2)$ → $d(x^2-y^2)/C(sp^2)^*$	0.1097	0.0977	0.1101	0.0853	0.0971	0.1276	0.1430
Sums of Weights							
Configuration	**25/15 CPCM**	**25/15 Gas**	**25/20 Gas**	**25/25 Gas**	**25/30 Gas**	**25/35 Gas**	**25/40 Gas**
CSS	58%	55%	53%	52%	50%	49%	47%
Sum of MLCT	23%	26%	25%	24%	23%	26%	25%
Sum of d-d	14%	13%	16%	19%	21%	21%	23%
Sum of MLCT+ d-d	3.4%	3.9%	2.6%	1.9%	1.7%	2.8%	2.8%
Singlet → Singlet Transition Energies (kcal mol^{-1})							
Transition	**25/15 CPCM**	**25/15 Gas**	**25/20 Gas**	**25/25 Gas**	**25/30 Gas**	**25/35 Gas**	**25/40 Gas**
$S_0 \rightarrow S_1$	42.6	38.0	39.3	40.1	40.6	39.3	39.8
$S_0 \rightarrow S_2$	47.3	42.5	43.3	43.7	43.9	43.2	43.4
$S_0 \rightarrow S_3$	52.3	47.3	48.0	48.9	49.5	48.2	48.3
$S_0 \rightarrow S_4$	64.3	59.6	60.9	62.1	62.6	61.2	61.7
$S_0 \rightarrow S_5$	64.9	60.5	61.9	62.5	63.0	61.8	62.1
$S_0 \rightarrow S_6$	65.4	61.7	62.3	63.4	63.4	63.2	63.0
$S_0 \rightarrow S_7$	70.2	65.1	67.7	67.7	67.3	68.0	67.9
$S_0 \rightarrow S_8$	71.3	66.7	68.6	69.2	69.0	68.4	68.1
$S_0 \rightarrow S_9$	71.5	69.4	68.8	70.1	70.3	69.4	69.7
$S_0 \rightarrow S_{10}$	72.3	72.2	71.1	70.6	70.7	71.3	71.7
$S_0 \rightarrow S_{11}$	73.3	73.4	71.8	72.0	72.5	72.0	72.0
$S_0 \rightarrow S_{12}$	77.0	75.0	73.0	72.1	73.4	72.2	72.7
$S_0 \rightarrow S_{13}$	78.2	76.2	74.5	74.5	75.2	75.7	74.2
$S_0 \rightarrow S_{14}$	85.6	81.2	80.9	81.5	81.7	81.7	81.4

Table S1G-2. Compound **1** – CASSCF/QD-NEVPT2 composition of the singlet 3.20 Å ground state while varying number of singlet roots. 9o, 10e Active Space – 25 triplet roots, *X* singlet roots (where *X* ranged from 15 to 45). Orbitals: bonding $d(x^2\text{-}y^2)/C(sp^2)$, d(xy), d(xz), d(yz), $d(z^2)$, $d(x^2\text{-}y^2)/C(sp^2)^*$, π*(1), π*(2), π*(3).

CI-Vector Weights (# Triplets/# Singlets)				
Transition	**25/15 CPCM**	**25/15 Gas**	**25/25 Gas**	**25/35 Gas**
$d(xz)$ + bonding $d(x^2\text{-}y^2)/C(sp^2)$ → $d(x^2\text{-}y^2)/C(sp^2)^*$ + π*(1)	0.5994	0.5998	0.6929	0.7298
d(xz) → π*(1)	0.1042	0.1057	0.0796	0.0626
bonding $d(x^2\text{-}y^2)/C(sp^2)$ → $d(x^2\text{-}y^2)/C(sp^2)^*$	0.0560	0.0567	0.0631	0.0663
$d(z^2)$ + d(xz) → $C(sp^2)$ + π*(1)	0.0579	0.0549	0.0195	0.0387

Singlet → Singlet Transition Energies (kcal mol^{-1})				
Transition	**25/15 CPCM**	**25/15 Gas**	**25/25 Gas**	**25/35 Gas**
$S_0 \rightarrow S_1$	42.6	38.0	40.1	39.3
$S_0 \rightarrow S_2$	47.3	42.5	43.7	43.2
$S_0 \rightarrow S_3$	52.3	47.3	48.9	48.2
$S_0 \rightarrow S_4$	64.3	59.6	62.1	61.2
$S_0 \rightarrow S_5$	64.9	60.5	62.5	61.8
$S_0 \rightarrow S_6$	65.4	61.7	63.4	63.2
$S_0 \rightarrow S_7$	70.2	65.1	67.7	68.0
$S_0 \rightarrow S_8$	71.3	66.7	69.2	68.4
$S_0 \rightarrow S_9$	71.5	69.4	70.1	69.4
$S_0 \rightarrow S_{10}$	72.3	72.2	70.6	71.3
$S_0 \rightarrow S_{11}$	73.3	73.4	72.0	72.0
$S_0 \rightarrow S_{12}$	77.0	75.0	72.1	72.2
$S_0 \rightarrow S_{13}$	78.2	76.2	74.5	75.7
$S_0 \rightarrow S_{14}$	85.6	81.2	81.5	81.7

Table S1G-3. Compound **1** – CASSCF/QD-NEVPT2 composition of the formal Ni(I) ground state while varying number of doublet roots. 8o, 9e Active Space – 25 quartet roots, *X* doublet roots (where *X* ranged from 15 to 45).

CI-Vector Weights (# Quartets / # Doublets)					
Transition	**25/15 CPCM**	**25/15 Gas**	**25/25 Gas**	**25/35 Gas**	**25/45 Gas**
d(xz) → π*(1)	0.7390	0.7363	0.7382	0.7701	0.7631
d(xz) → π*(2)	0.0761	0.0755	0.0746	0.0710	0.0719
formal Ni(I)	0.0733	0.0727	0.0724	0.0716	0.0748
d(yz) → π*(3)	0.0428	0.0455	0.0474	0.0443	0.0467

Doublet→Doublet Transition Energies (kcal mol^{-1})					
Transition	**25/15 CPCM**	**25/15 Gas**	**25/25 Gas**	**25/35 Gas**	**25/45 Gas**
1	8.3	9.4	9.4	9.6	9.8
2	11.9	12.7	12.7	12.9	13.1
3	22.5	23.0	22.3	22.5	22.7
4	26.5	26.6	26.6	26.9	27.0
5	27.6	28.2	26.8	27.2	27.5
6	29.4	30.3	30.4	30.1	30.1
7	31.0	31.0	30.6	30.6	30.8
8	33.7	34.3	34.3	34.5	34.9
9	35.2	36.0	36.2	36.4	36.7
10	36.5	37.7	37.4	37.7	37.9
11	36.7	38.1	37.6	37.7	38.0
12	37.8	38.3	38.0	38.4	38.8
13	37.9	38.4	38.3	38.6	39.0
14	49.3	48.1	45.7	46.1	45.9

Table S1H. Compound **1** – CASSCF/QD-NEVPT2. Transitions for the gas phase spectrum. 9o, 10e Active Space – 25 triplet roots, 15 singlet roots. Orbitals (in order for CI vector notation below): d(xy), bonding d(x^2-y^2)/C(sp^2), d(yz), d(z^2), d(xz), d(x^2-y^2)/C(sp^2)*, π*(1), π*(2), π*(3).

Transition	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
$S_0 \rightarrow S_1$	752.5	38.0	222120100	0.0006862	0.8166
			202122100	---	0.0850
$S_0 \rightarrow S_2$	672.0	42.5	221220100	0.0649528	0.4507
			222210100	---	0.2848
$S_0 \rightarrow S_3$	604.1	47.3	221220100	0.1224866	0.3511
			222210100	---	0.2756
$S_0 \rightarrow S_4$	479.5	59.6	222120010	0.0003566	0.7222
			202122010	---	0.0773
$S_0 \rightarrow S_5$	472.4	60.5	122220100	0.0001327	0.7056
			221211100	---	0.0791
$S_0 \rightarrow S_6$	463.2	61.7	222210010	0.0858212	0.3931
			221220010	---	0.2037
$S_0 \rightarrow S_7$	439.3	65.1	222120001	0.0000514	0.7108
			202122001	---	0.0744
$S_0 \rightarrow S_8$	428.4	66.7	221220010	0.0799110	0.3735
			222210001	---	0.3188
$S_0 \rightarrow S_9$	411.9	69.4	222210001	0.1256711	0.2387
			221220010	---	0.2186
$S_0 \rightarrow S_{10}$	396.2	72.2	222211000	0.0001096	0.7697
			212212000	---	0.0922
$S_0 \rightarrow S_{11}$	389.3	73.4	122221000	0.0146636	0.6323
			122211100	---	0.0868
$S_0 \rightarrow S_{12}$	381.1	75.0	221221000	0.0008472	0.7203
			211222000	---	0.0560
$S_0 \rightarrow S_{13}$	375.2	76.2	222121000	0.1025873	0.4292
			222210001	---	0.1754
$S_0 \rightarrow S_{14}$	351.9	81.2	221220001	0.4703139	0.5884
			212221000	---	0.0772

Table S1I-1. Compound **1** – CASSCF/QD-NEVPT2. Transitions for the CPCM(THF) phase spectrum. 9o, 10e Active Space – 25 triplet roots, 15 singlet roots. Orbital (in order for CI vector notation below): d(xy), bonding $d(x^2-y^2)/C(sp^2)$, d(yz), d(xz), $d(z^2)$, $d(x^2-y^2)/C(sp^2)$*, π*(1), π*(2), π*(3).

Transition	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
$S_0 \rightarrow S_1$	671.4	42.6	222210100	0.0008408	0.8161
			202212100	---	0.0876
$S_0 \rightarrow S_2$	604.2	47.3	221220100	0.0622469	0.4193
			222120100	---	0.3382
$S_0 \rightarrow S_3$	546.6	52.3	221220100	0.1520657	0.3722
			222120100	---	0.2674
$S_0 \rightarrow S_4$	444.6	64.3	222120010	0.1043472	0.5270
			221220010	---	0.1267
$S_0 \rightarrow S_5$	440.4	64.9	122220100	0.0001963	0.4135
			222210010	---	0.3424
$S_0 \rightarrow S_6$	437.3	65.4	222210010	0.0003333	0.4320
			122220100	---	0.3239
$S_0 \rightarrow S_7$	407.1	70.2	222121000	0.0002537	0.6733
			221221000	---	0.1149
$S_0 \rightarrow S_8$	401.3	71.3	222211000	0.0305023	0.2808
			221220010	---	0.2155
$S_0 \rightarrow S_9$	399.9	71.5	122221000	0.0329884	0.4648
			222211000	---	0.1385
$S_0 \rightarrow S_{10}$	395.3	72.3	222210001	0.0001302	0.7121
			202212001	---	0.0765
$S_0 \rightarrow S_{11}$	390.1	73.3	221221000	0.0016152	0.5853
			222121000	---	0.1189
$S_0 \rightarrow S_{12}$	371.3	77.0	221220010	0.0139708	0.3376
			222211000	---	0.2166
$S_0 \rightarrow S_{13}$	365.5	78.2	222120001	0.1967238	0.4902
			222211000	---	0.0927
$S_0 \rightarrow S_{14}$	333.9	85.6	221220001	0.4607820	0.6454
			212221000	---	0.0665

Table S1I-2. Compound **1** – CASSCF/QD-NEVPT2. Spin-orbit corrected absorption transitions for the CPCM(THF) phase spectrum. 9o, 10e Active Space – 25 triplet roots, 15 singlet roots.

Energy/ nm	**Energy/ kcal mol^{-1}**	f_{osc}	**Energy/ nm**	**Energy/ kcal mol^{-1}**	f_{osc}
686.8	41.6	0.0006638	420.9	67.9	0.0026607
681.3	42.0	0.0000492	420.7	68.0	0.0000932
679.1	42.1	0.0014753	413.2	69.2	0.0153295
672.4	42.5	0.0018573	412.5	69.3	0.0001385
641.0	44.6	0.0000800	412.5	69.3	0.0028688
640.3	44.7	0.0022972	405.7	70.5	0.0001127
638.3	44.8	0.0002073	398.7	71.7	0.0002244
602.4	47.5	0.0625017	398.2	71.8	0.0400852
567.6	50.4	0.0000177	397.7	71.9	0.0078340
566.9	50.4	0.0003588	389.3	73.4	0.0017359
566.5	50.5	0.0056594	381.8	74.9	0.0000093
548.2	52.2	0.0000804	381.7	74.9	0.0007565
548.0	52.2	0.0000025	381.7	74.9	0.0000361
547.4	52.2	0.0077188	378.1	75.6	0.0000159
541.3	52.8	0.1271535	377.9	75.6	0.0081108
453.0	63.1	0.0581791	377.2	75.8	0.0001353
446.5	64.0	0.0000000	369.9	77.3	0.0213533
446.4	64.1	0.0013619	364.8	78.4	0.1646061
444.2	64.4	0.0002830	350.5	81.6	0.0000067
437.0	65.4	0.0000814	350.3	81.6	0.0222811
434.5	65.8	0.0442016	350.2	81.6	0.0000361
422.4	67.7	0.0020976	332.2	86.1	0.4457060

Table S1J. Compound **1** – TDDFT calculated lowest transition energies with CPCM(THF).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	Transition	f_{osc}	Contribution
0	0	1	---	---	---	---	---
					---	---	---
1	1	3	858.5	33.3	119a → 123a	---	0.77795
					118a → 123a	---	0.13713
2	2	3	745.4	38.4	117a → 123a	---	0.70862
					118a → 123a	---	0.10691
3	5	3	689.5	41.4	119a → 120a	---	0.86068
					118a → 120a	---	0.09258
4	3	3	677.1	42.2	116a → 123a	---	0.76487
					115a → 123a	---	0.08395
5	8	3	660.6	43.3	118a → 120a	---	0.74196
					117a → 120a	---	0.11865
6	6	3	613.9	46.6	117a → 120a	---	0.81309
					118a → 120a	---	0.12652
7	14	3	593.8	48.1	115a → 120a	---	0.70784
					114a → 120a	---	0.13833
8	1	1	580.6	49.2	119a → 120a	0.0008793	0.85637
					118a → 120a	---	0.08983
9	4	3	530.2	53.9	114a → 123a	---	0.48094
					109a → 123a	---	0.16890
10	7	3	504.4	56.7	116a → 120a	---	0.85548
					115a → 120a	---	0.07395
11	9	3	504.2	56.7	114a → 120a	---	0.76732
					115a → 120a	---	0.16764
12	2	1	486.4	58.8	119a → 123a	0.0149377	0.43727
					117a → 120a	---	0.28572
13	11	1	464.3	61.6	115a → 120a	0.0010048	0.74526
					114a → 120a	---	0.17279
14	10	3	456.9	62.6	113a → 120a	---	0.81346
					114a → 120a	---	0.04189
15	3	1	451.4	63.3	117a → 123a	0.0000160	0.69793
					118a → 123a	---	0.09923
16	17	3	451.4	63.3	118a → 121a	---	0.71600
					117a → 121a	---	0.11668
17	4	1	438.8	65.2	117a → 120a	0.0091056	0.31383
					119a → 123a	---	0.20057
18	5	1	438.8	65.2	118a → 120a	0.0000671	0.34012
					116a → 123a	---	0.33024
19	6	1	432.3	66.1	116a → 123a	0.0006521	0.39229
					118a → 120a	---	0.30750
20	9	1	429.6	66.5	114a → 120a	0.0002344	0.74666
					115a → 120a	---	0.16061

Table S1K. Compound **1** – TDDFT with CPCM(THF). Transitions corresponding to singlets down to 300 nm.

Root	ΔE/nm	ΔE/kcal mol^{-1}	Transition	f_{osc}	Contribution
1	580.6	49.2	119a → 120a	0.0008793	0.85637
			118a → 120a	---	0.08983
2	486.4	58.8	119a → 123a	0.0149377	0.43727
			117a → 120a	---	0.28572
11	464.3	61.6	115a → 120a	0.0010048	0.74526
			114a → 120a	---	0.17279
3	451.4	63.3	117a → 123a	0.0000160	0.69793
			118a → 123a	---	0.09923
4	438.8	65.2	117a → 120a	0.0091056	0.31383
			119a → 123a	---	0.20057
5	438.8	65.2	118a → 120a	0.0000671	0.34012
			116a → 123a	---	0.33024
6	432.3	66.1	116a → 123a	0.0006521	0.39229
			118a → 120a	---	0.30750
9	429.6	66.5	114a → 120a	0.0002344	0.74666
			115a → 120a	---	0.16061
8	429.3	66.6	116a → 120a	0.0774053	0.73096
			117a → 120a	---	0.11234
7	416.4	68.7	114a → 123a	0.0040780	0.43475
			109a → 123a	---	0.10090
10	411.7	69.4	119a → 121a	0.0002556	0.90253
			118a → 121a	---	0.06081
14	393.7	72.6	118a → 121a	0.0002484	0.74852
			117a → 121a	---	0.13455
13	374.9	76.3	119a → 122a	0.0000090	0.88873
			118a → 122a	---	0.07966
12	372.2	76.8	117a → 121a	0.0103918	0.75836
			118a → 121a	---	0.13533
18	363.5	78.7	118a → 122a	0.0002226	0.72376
			117a → 122a	---	0.11295
21	343.8	83.2	115a → 121a	0.0293580	0.61427
			114a → 121a	---	0.22459
17	341.1	83.8	116a → 121a	0.0253815	0.72971
			117a → 122a	---	0.10940
16	339.9	84.1	112a → 120a	0.0000921	0.96045
			---	---	---
15	335.0	85.4	117a → 122a	0.0228657	0.61108
			116a → 121a	---	0.12381
19	334.8	85.4	114a → 121a	0.0004394	0.68195
			115a → 121a	---	0.24704
25	321.7	88.9	115a → 122a	0.0021238	0.61609
			114a → 122a	---	0.16497

Table S1L. Compound **1** with Ni–C distance of 3.20 Å – CASSCF/QD-NEVPT2 lowest transition energies in CPCM(THF). 8o, 10e Active Space – 25 triplet roots, 15 singlet roots. Orbitals (in order for CI vector notation below): d(xy), d(yz), d(z^2), d(xz), bonding d(x^2-y^2)/C(sp^2), d(x^2-y^2)/C(sp^2)*, π*(1), π*(2).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
0	0	1	---	---	22211110	---	0.5994
					22212010	---	0.1042
					22112110	---	0.0579
1	0	3	9220.8	3.1	22211110	---	0.7413
					22112110	---	0.0631
2	1	3	4238.2	6.8	22121110	---	0.8175
					22122010	---	0.1200
3	1	1	3665.3	7.8	22121110	0.0000056	0.8154
					22122010	---	0.1208
4	2	3	3436.2	8.3	22211110	---	0.7508
					22212010	---	0.0904
5	3	3	2779.3	10.3	22121110	---	0.9893
					12221110	---	0.0030
6	4	3	2465.5	11.6	21221110	---	0.7577
					21222010	---	0.1076
7	2	1	2439.5	11.7	21221110	0.0000012	0.6968
					21222010	---	0.1037
8	5	3	2034.0	14.1	21221110	---	0.8601
					22211110	---	0.0519
9	3	1	1185.6	24.1	22220110	0.0001996	0.7437
					22221010	---	0.0721
10	6	3	1184.1	24.1	22220110	---	0.7898
					22221010	---	0.0749
11	4	1	1117.7	25.6	22211101	0.0501900	0.6199
					22212001	---	0.0954
12	5	1	1102.6	25.9	21212110	0.0046113	0.3668
					12221110	---	0.3589
13	7	3	1070.5	26.7	12221110	---	0.4548
					21212110	---	0.4330
14	8	3	1050.9	27.2	22121101	---	0.8032
					22122001	---	0.1181
15	9	3	1043.3	27.4	22211101	---	0.7337
					22212001	---	0.0821
16	6	1	1042.0	27.4	22121101	0.0000466	0.8118
					22122001	---	0.1196
17	10	3	1008.1	28.4	12221110	---	0.4842
					21212110	---	0.4145
18	11	3	994.2	28.8	22211101	---	0.8211
					22112101	---	0.0703
19	12	3	960.4	29.8	22121101	---	0.9873
					12221101	---	0.0030
20	7	1	896.2	31.9	21221101	0.0028482	0.7468
					21222001	---	0.1085

Table S1M. Compound **1** – CASSCF/QD-NEVPT2 composition of the singlet equilibrium ground state with Ni–C distance of 3.20 Å – CASSCF/QD-NEVPT2 in gas phase. 8o, 10e Active Space – 25 triplet roots, 15 singlet roots. Orbitals (in order for CI vector notation below): d(xy), d(yz), $d(z^2)$, d(xz), bonding $d(x^2\text{-}y^2)/C(sp^2)$, $d(x^2\text{-}y^2)/C(sp^2)^*$, π*(1), π*(2).

CI Vector	Transition	Contribution
22211110	d(xz) + bonding $d(x^2\text{-}y^2)/C(sp^2)$ → $d(x^2\text{-}y^2)/C(sp^2)^*$ + π*(1)	0.5998
22212010	d(xz) → π*(1)	0.1057
22221100	bonding $d(x^2\text{-}y^2)/C(sp^2)$ → $d(x^2\text{-}y^2)/C(sp^2)^*$	0.0567
22112110	d(xz) + $d(z^2)$ → $d(x^2\text{-}y^2)/C(sp^2)^*$ + π*(1)	0.0549
22210210	d(xz) + 2x[bonding $d(x^2\text{-}y^2)/C(sp^2)$] → 2x[$d(x^2\text{-}y^2)/C(sp^2)^*$] + π*(1)	0.0472
21221110	d(yz) + bonding $d(x^2\text{-}y^2)/C(sp^2)$ → $d(x^2\text{-}y^2)/C(sp^2)^*$ + π*(1)	0.0434
22211101	d(xz) + bonding $d(x^2\text{-}y^2)/C(sp^2)$ → $d(x^2\text{-}y^2)/C(sp^2)^*$ + π*(2)	0.0273
11222110	d(yz) + d(xy) → $d(x^2\text{-}y^2)/C(sp^2)^*$ + π*(1)	0.0170
22222000	Closed shell singlet (CSS) d^8	0.0105
21222010	d(yz) → π*(1)	0.0067
22212001	d(xz) → π*(2)	0.0047
22122100	$d(z^2)$ → $d(x^2\text{-}y^2)/C(sp^2)^*$	0.0034
21220210	2x[bonding $d(x^2\text{-}y^2)/C(sp^2)$] + d(yz) → 2x[$d(x^2\text{-}y^2)/C(sp^2)^*$] + π*(1)	0.0034
12212110	d(xy) + d(xz) → $d(x^2\text{-}y^2)/C(sp^2)^*$ + π*(1)	0.0032

Table S1N. Compound **1** – CASSCF/QD-NEVPT2 composition of the singlet equilibrium ground state with Ni–C distance of 3.20 Å – CASSCF/QD-NEVPT2 with CPCM(THF). 8o, 10e Active Space – 25 triplet roots, 15 singlet roots. Orbitals (in order for CI vector notation below): d(xy), d(yz), $d(z^2)$, d(xz), bonding $d(x^2\text{-}y^2)/C(sp^2)$, $d(x^2\text{-}y^2)/C(sp^2)^*$, π*(1), π*(2).

CI Vector	Transition	Contribution
22211110	d(xz) + bonding $d(x^2\text{-}y^2)/C(sp^2)$ → $d(x^2\text{-}y^2)/C(sp^2)^*$ + π*(1)	0.5994
22212010	d(xz) → π*(1)	0.1042
22112110	d(xz) + $d(z^2)$ → $d(x^2\text{-}y^2)/C(sp^2)^*$ + π*(1)	0.0579
22221100	bonding $d(x^2\text{-}y^2)/C(sp^2)$ → $d(x^2\text{-}y^2)/C(sp^2)^*$	0.0560
21221110	d(yz) + bonding $d(x^2\text{-}y^2)/C(sp^2)$ → $d(x^2\text{-}y^2)/C(sp^2)^*$ + π*(1)	0.0463
22210210	d(xz) + 2x[bonding $d(x^2\text{-}y^2)/C(sp^2)$] → 2x[$d(x^2\text{-}y^2)/C(sp^2)^*$] + π*(1)	0.0463
22211101	d(xz) + bonding $d(x^2\text{-}y^2)/C(sp^2)$ → $d(x^2\text{-}y^2)/C(sp^2)^*$ + π*(2)	0.0254
11222110	d(yz) + d(xy) → $d(x^2\text{-}y^2)/C(sp^2)^*$ + π*(1)	0.0169
22222000	Closed shell singlet (CSS) d^8	0.0102
21222010	d(yz) → π*(1)	0.0071
22212001	d(xz) → π*(2)	0.0043
22122100	$d(z^2)$ → $d(x^2\text{-}y^2)/C(sp^2)^*$	0.0035
21220210	2x[bonding $d(x^2\text{-}y^2)/C(sp^2)$] + d(yz) → 2x[$d(x^2\text{-}y^2)/C(sp^2)^*$] + π*(1)	0.0035
12212110	d(xy) + d(xz) → $d(x^2\text{-}y^2)/C(sp^2)^*$ + π*(1)	0.0029

Table S1O. Leadings terms of CI-vector for T_0 (first triplet manifold reached from vertical excitation of singlet ground state) of **1** in Figure 4. In the vicinity of the equilibrium geometry, the CI-vector is dominated by ^{3}d-d transitions. Note that using the relaxed, DFT optimized T_d triplet geometries of **1** (surfaces shown in Figure 1) the ground state triplet CI-vector is very heavily dominated by the $[d(x^2\text{-}y^2)]^1[d(z^2)/C(sp^2)^*]^1$ ^{3}d-d configuration (65% at the 1.9 Å equilibrium geometry, Figure S1H). For T_0, at long Ni–C distances, the transition d(xz) → π*(1) is very dominant, but still less so than in the repulsive manifold shown in black, and assigned to the aforementioned transition, in Figure 4.

Ni–C Distance (Å)	Weight	Transition
1.60	0.8420	$d(z^2) \rightarrow \pi^*(1)$
	0.0669	$d(xy) \rightarrow \pi^*(1)$
1.80	0.7339	$d(z^2) \rightarrow \pi^*(1)$
	0.0867	$d(xy) \rightarrow \pi^*(1)$
1.89 (equil.)	0.4035	$d(z^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$
	0.1917	$d(xz) \rightarrow \pi^*(1)$
2.20	0.4499	$d(xz) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$
	0.1777	$d(yz) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$
2.40	0.5278	$d(z^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$
	0.2942	$d(z^2)$ + bonding $d(x^2\text{-}y^2)/C(sp^2) \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*]$
2.60	0.4220	$dz2 \rightarrow \pi^*(1)$
	0.4045	$d(z^2)$ + bonding $d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$
2.80	0.5427	d(xz) + bonding $d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$
	0.2368	$d(xz) \rightarrow \pi^*(1)$
3.00	0.6998	d(xz) + bonding $d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$
	0.0650	$d(xz) \rightarrow \pi^*(1)$
3.20	0.7446	d(xz) + bonding $d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$
	0.0600	$d(z^2)$ + bonding $d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$
3.40	0.7572	d(xz) + bonding $d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$
	0.0610	bonding $d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$
3.60	0.7627	d(xz) + bonding $d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$
	0.0617	bonding $d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$

Table S1P. Spin Contamination Values From BSS Calculation and Yamaguchi Correction[1,2] BSS Energy of **1**. Using $\langle S^2 \rangle$ values and energies for the triplet and BSS solutions for the same geometry, $\alpha = \langle S^2 \rangle_{trip.}/(\langle S^2 \rangle_{trip.} - \langle S^2 \rangle_{BSS})$, $\beta = \langle S^2 \rangle_{BSS}/(\langle S^2 \rangle_{trip.} - \langle S^2 \rangle_{BSS})$, and $E_{Yamaguchi} = \alpha E_{BSS} - \beta E_{trip}$.

Ni–C Dist. (Å)	$\langle S^2 \rangle$ S=1	$\langle S^2 \rangle$ BSS	α	β	Energy S=1/ kcal mol^{-1}	Energy BSS/ kcal mol^{-1}	Energy Yamaguchi/ kcal mol^{-1}
1.60	2.01	0.00	1.00	0.00	72.8	22.4	22.4
1.80	2.01	0.00	1.00	0.00	43.6	1.9	1.9
1.89	2.01	0.00	1.00	0.00	38.3	0.0	0.0
2.00	2.01	0.00	1.00	0.00	35.8	1.1	1.1
2.20	2.01	0.00	1.00	0.00	37.2	8.2	8.2
2.40	2.01	0.00	1.00	0.00	42.0	17.8	17.8
2.60	2.02	0.24	1.13	0.13	47.0	27.3	24.7
2.80	2.03	0.51	1.34	0.34	48.1	34.0	29.1
3.00	2.03	0.71	1.53	0.53	47.0	38.2	33.5
3.20	2.03	0.83	1.70	0.70	46.2	40.9	37.1
3.40	2.03	0.92	1.82	0.82	45.5	42.4	39.9
3.60	2.03	0.96	1.91	0.91	45.0	43.3	41.7

C. Figures Part 1: Compound *1*

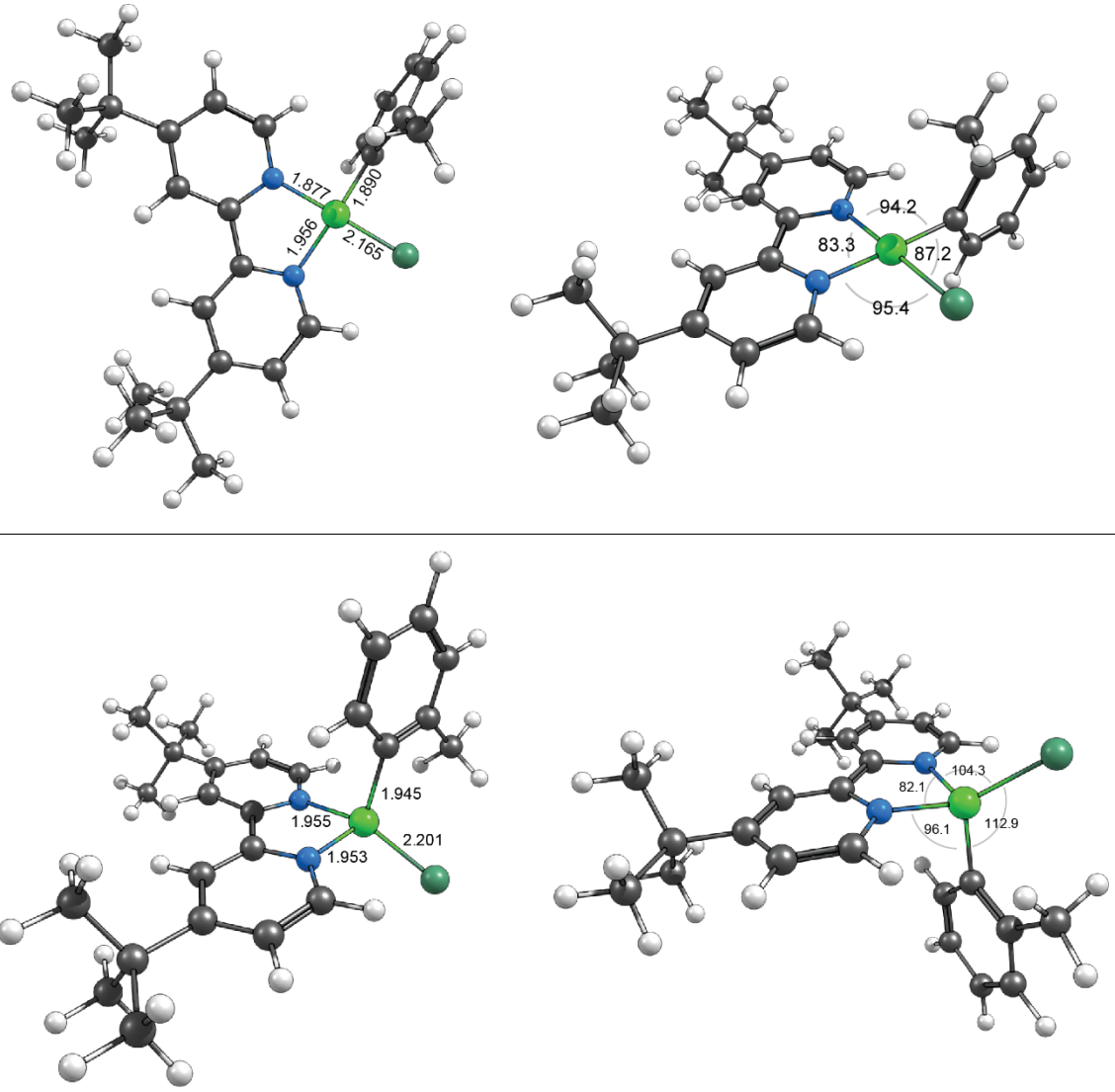


Figure S1A. Top: square planar equilibrium geometry of compound **1** (S=0), and bottom: tetrahedral equilibrium geometry of **1** (S=1) as calculated by DFT. Selected bond lengths and angles are shown.

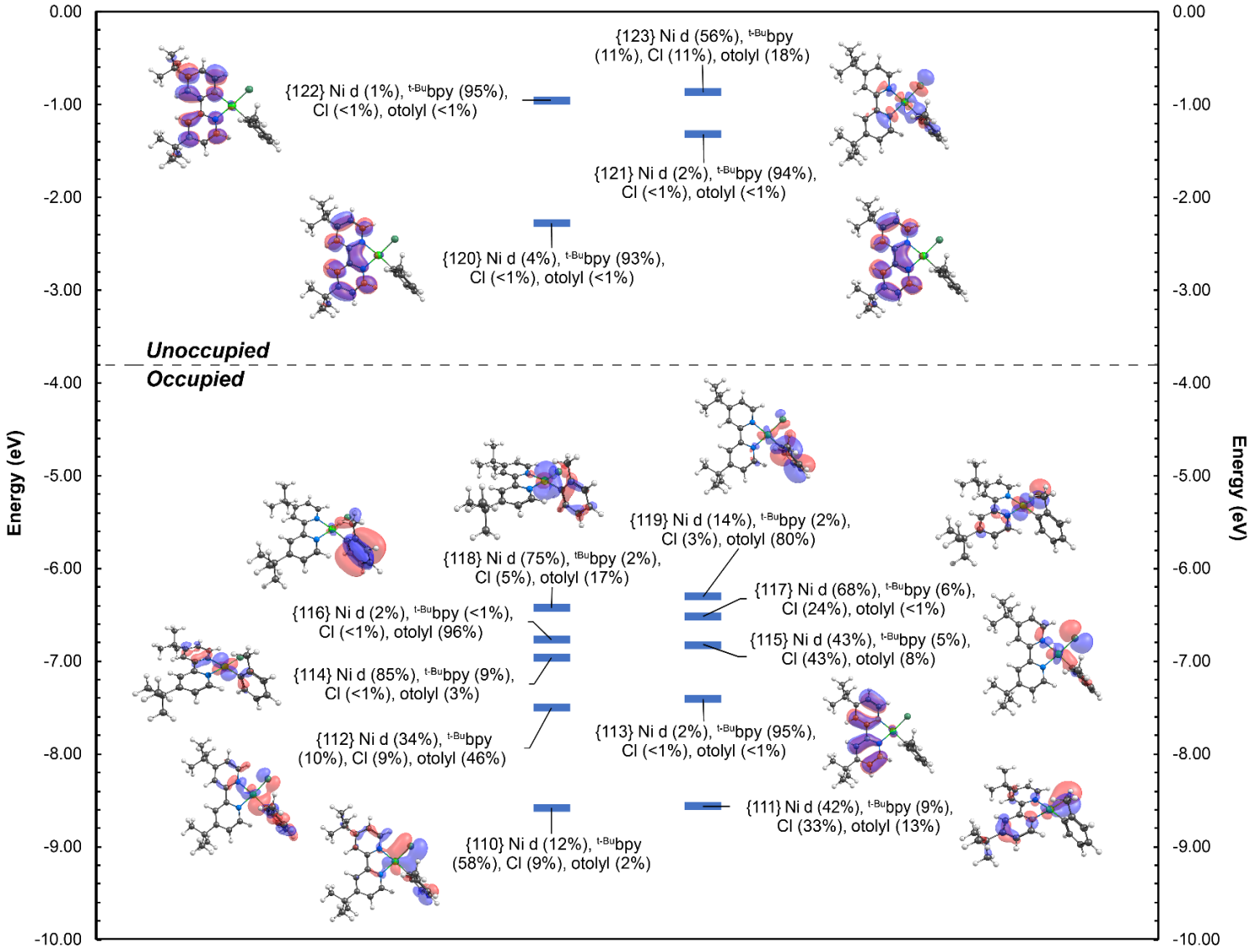


Figure S1B. Compound **1** (S=0) – Single point DFT frontier molecular orbital diagram. Orbitals are offset for clarity.

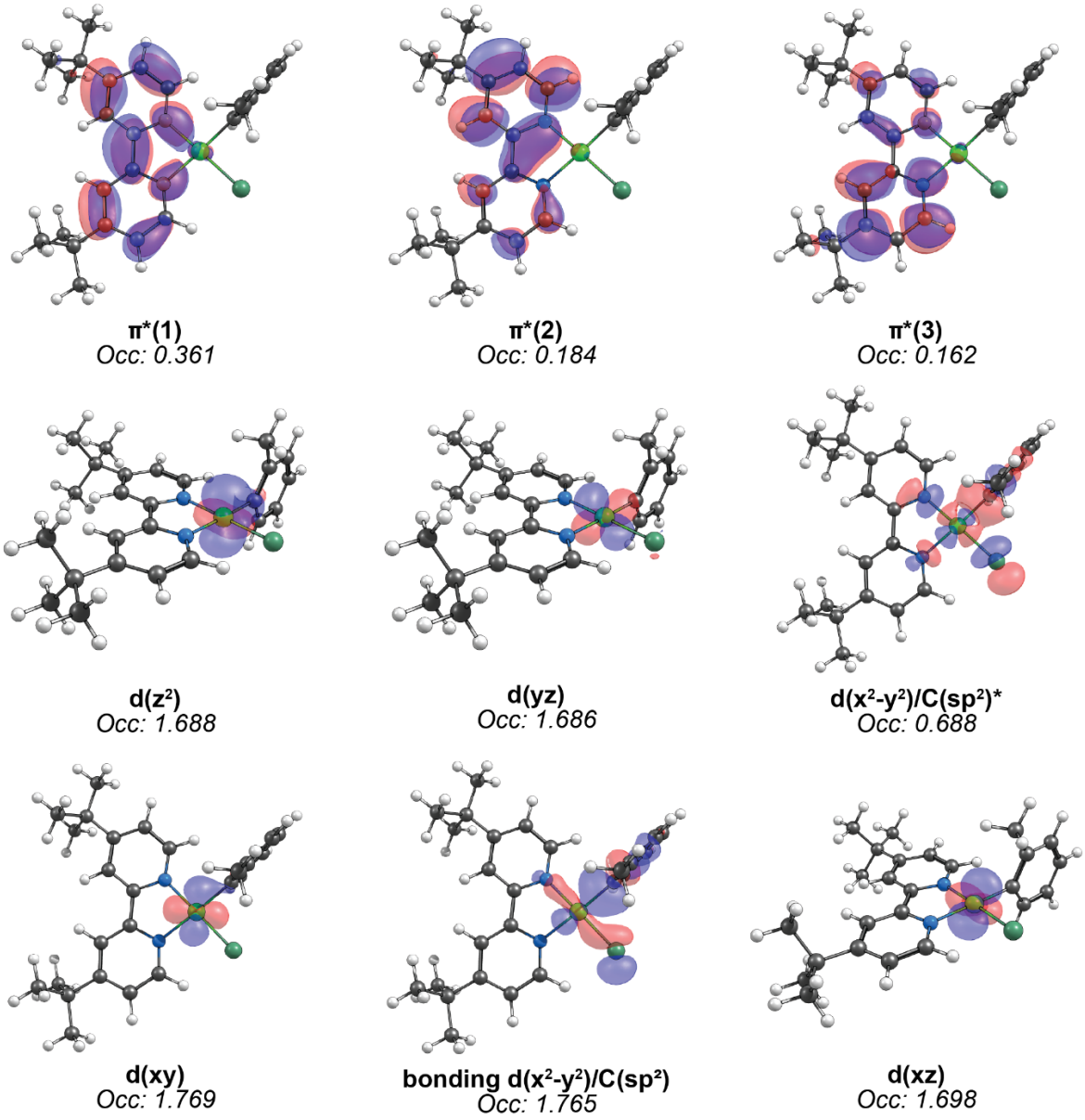


Figure S1C. Compound **1** (S=0) – CASSCF/QD-NEVPT2 9o, 10e Active Space.

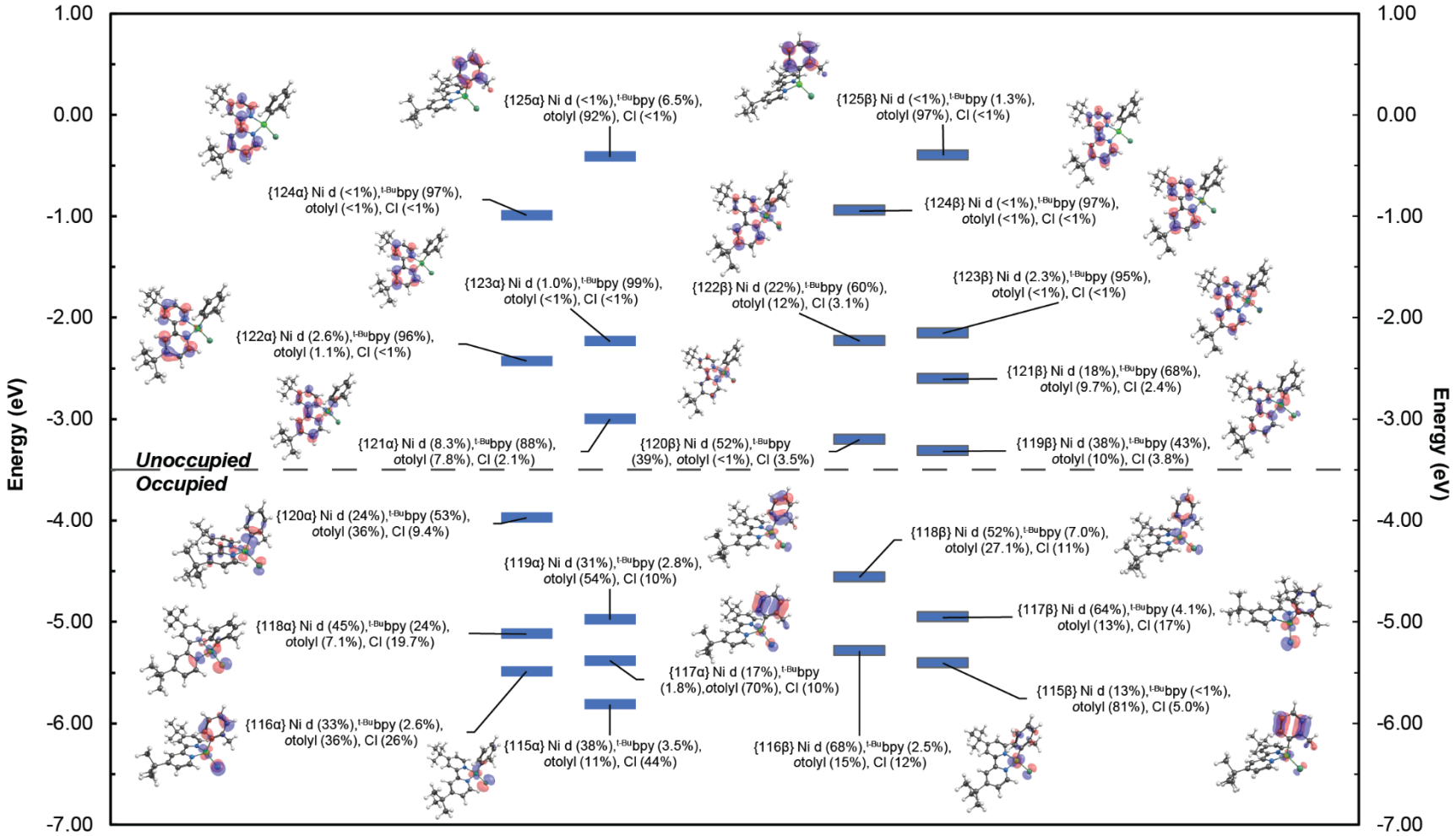


Figure S1D. Compound **1** (S=1) – Single point DFT frontier molecular orbital diagram, with α orbitals on the left and β orbitals on the right. α and β orbitals are also offset for clarity.

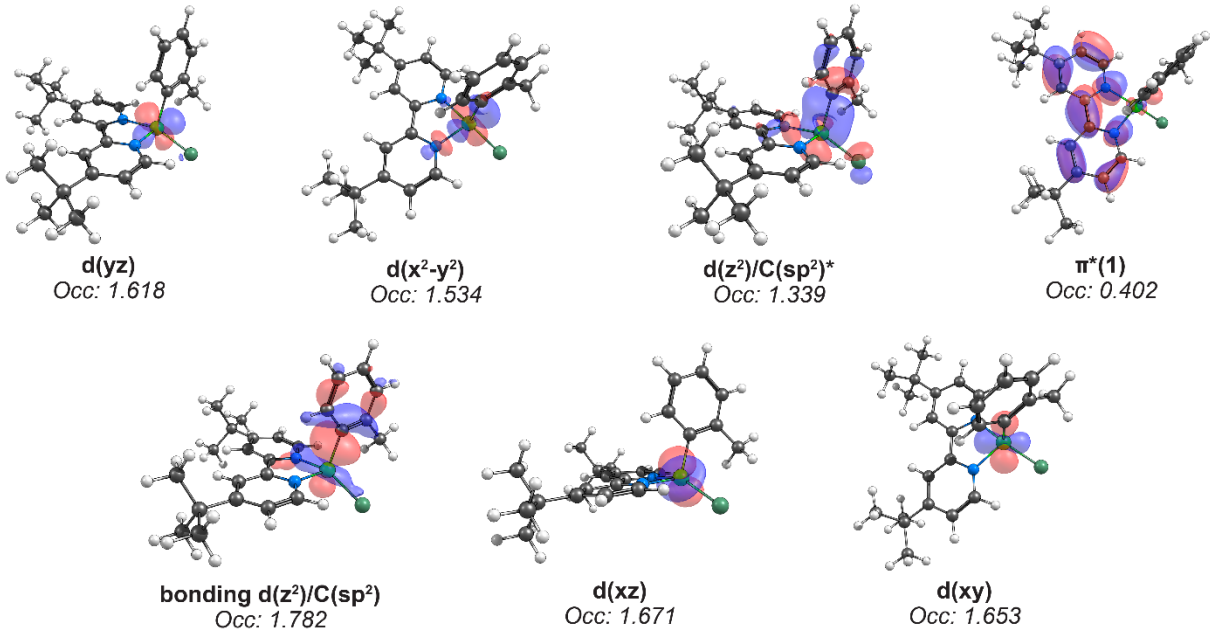


Figure S1E. Compound **1** (S=1) – CASSCF/QD-NEVPT2 7o, 10e Active Space.

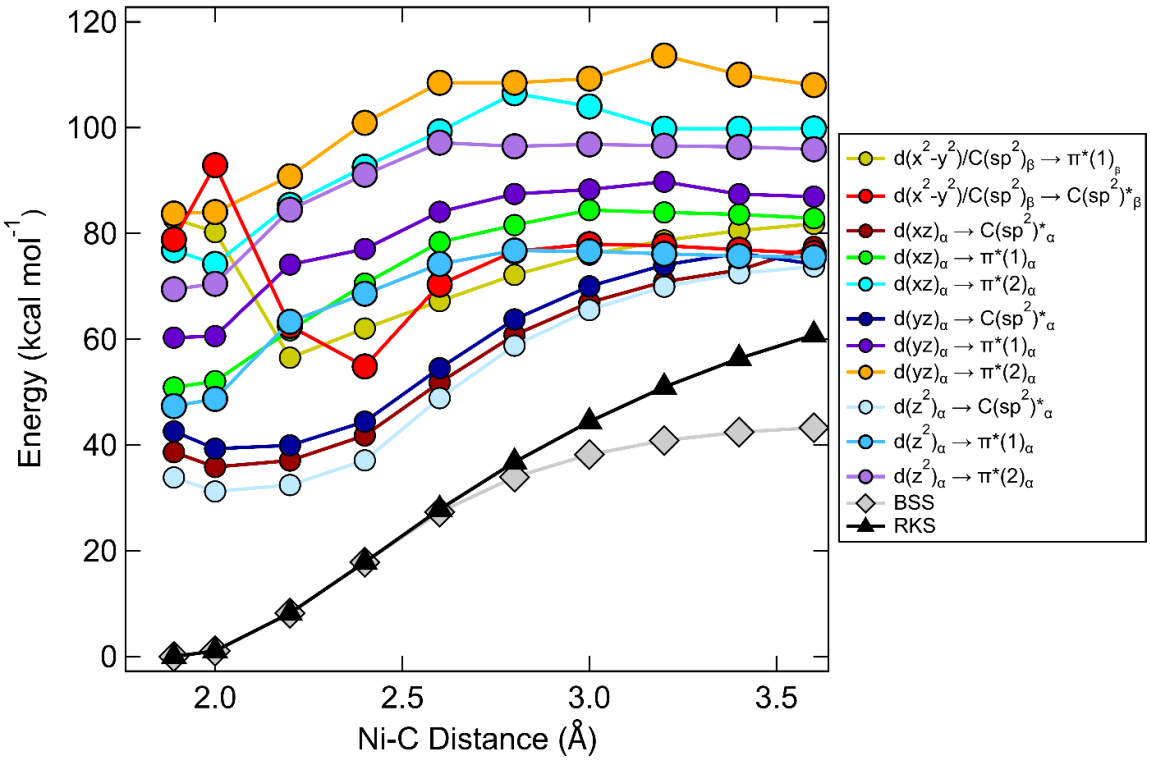


Figure S1F. Broken symmetry singlet TDDFT excitations along the Ni–C coordinate of **1** show no repulsive excited states. Spin-contaminated BSS calculations gave a Ni–C BDE of 43.3 kcal mol^{-1}, while the Yamaguchi corrected Ni–C BDE is only marginally different, at 41.7 kcal mol^{-1}.

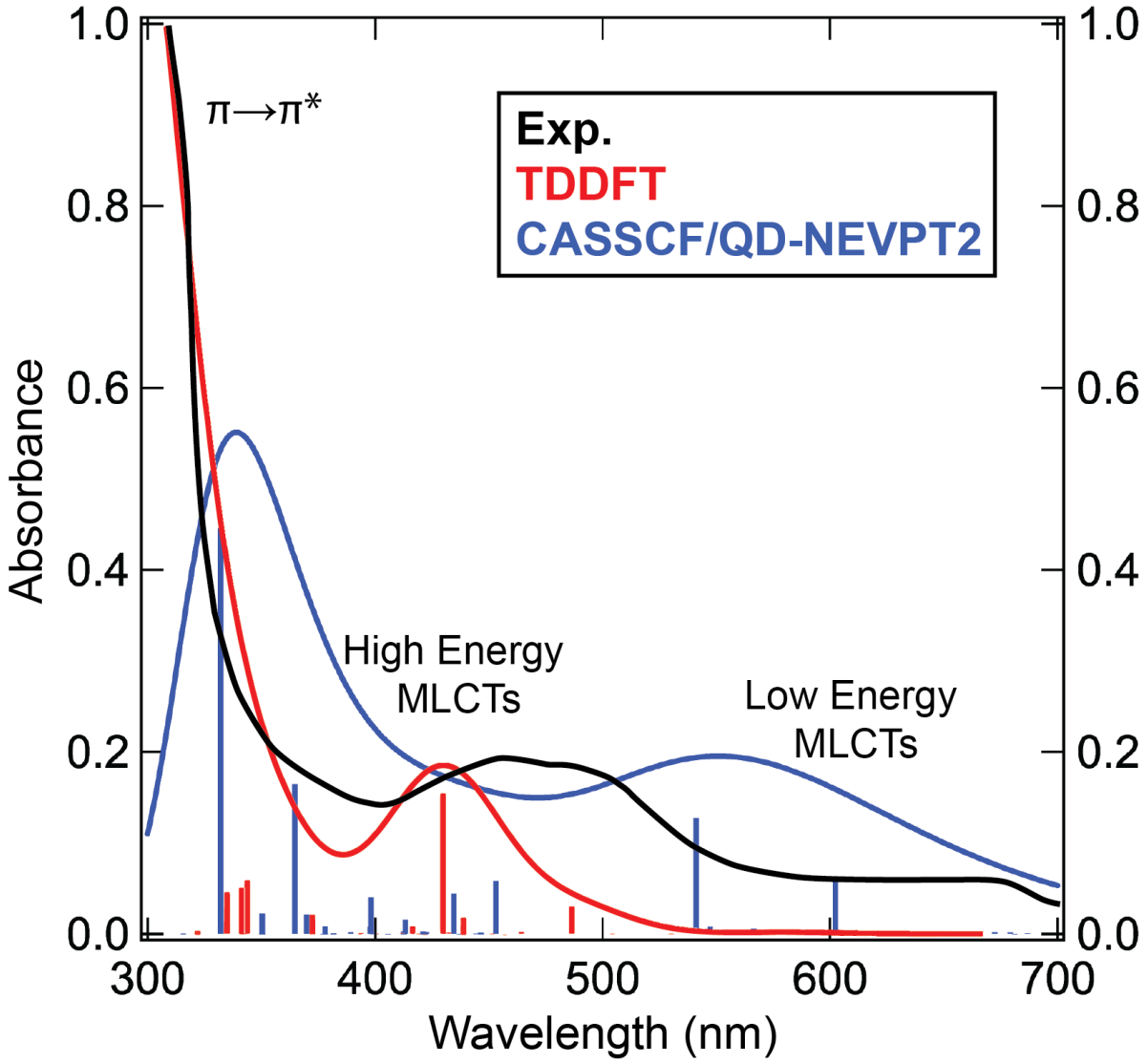


Figure S1G. Overlay of the experimental (THF) and calculated UV-vis spectrum of the equilibrium structure of **1**. The TDDFT calculated spectrum (CPCM(THF)) in this research aligns well with that previously reported.[3] The CASSCF/QD-NEVPT2 spectrum is spin-orbit coupling corrected with CPCM(THF). Note the relative oscillator strengths of the lower energy MLCT transitions are partially over-estimated in the CASSCF/QD-NEVPT2 calculated spectrum. This spectrum also does not display the intramolecular bpy-based π→π* transitions, as the π orbitals are not part of the active space.

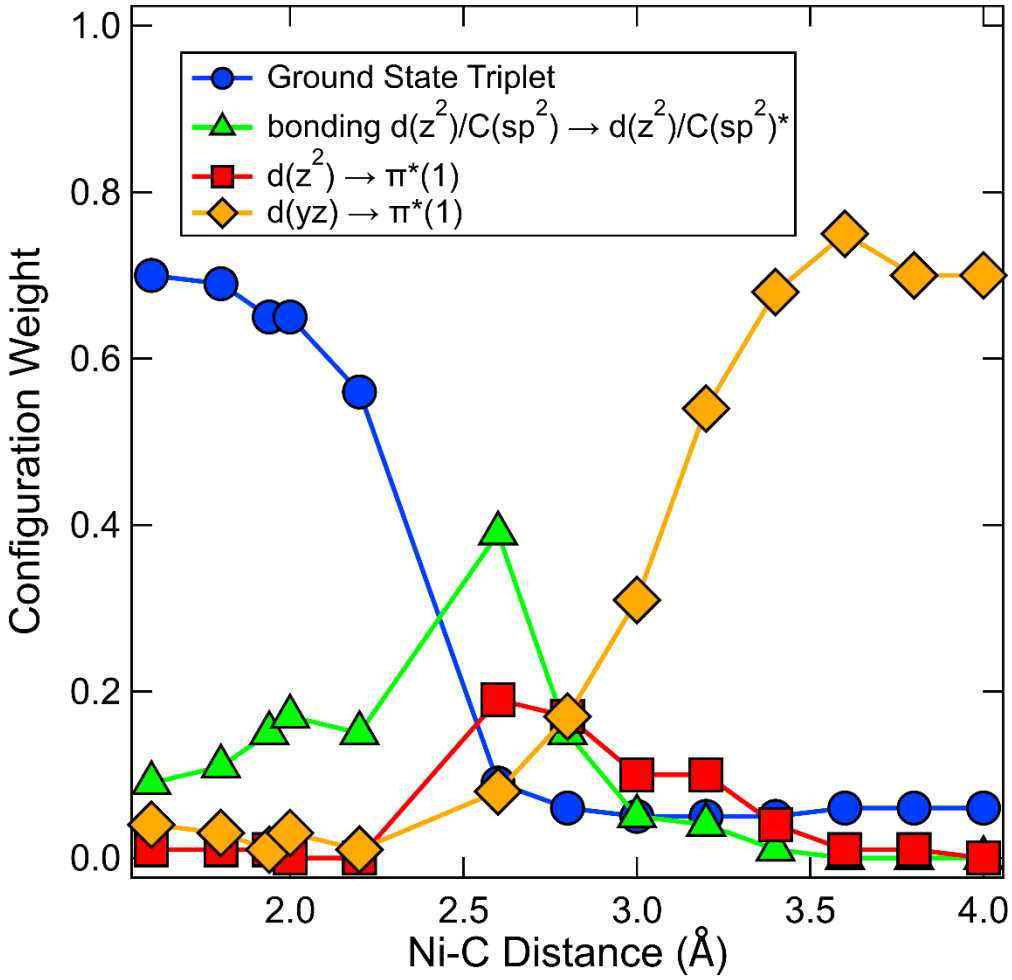


Figure S1H. Plot of the dominant configurations that contribute to the ground state CI vector along the optimized triplet Ni–C bond elongation surface of **1**. Note that for high spin **1**, the ground state triplet is $[d(x^2\text{-}y^2)]^1[(dz^2)/C(sp^2)^*]^1$, making a d(yz) → π*(1) transition yield an orbital configuration of $[d(yz)]^1[d(x^2\text{-}y^2)]^1[(dz^2)/C(sp^2)^*]^1[\pi^*(1)]^1$.

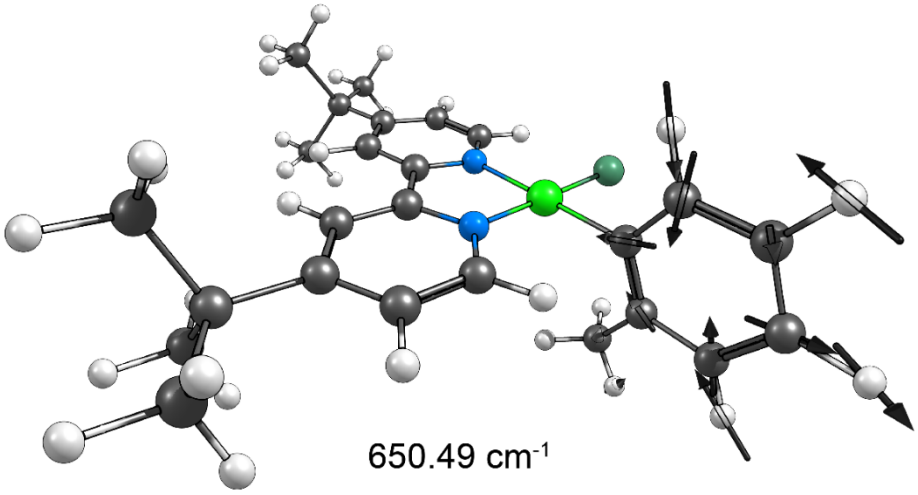


Figure S1I. Higher energy vibrational frequency in **1** that exhibits a Ni–C bond stretching mode.

D. Tables Part 2: Compound *2*

Table S2A. Compound **2** – TDDFT lowest transition energies with CPCM(THF).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	Transition	f_{osc}	Contribution
0	0	1	---	---	---	---	---
					---	---	---
1	1	3	869.2	32.9	90a → 94a	---	0.88196
					84a → 94a	---	0.03221
2	4	3	840.6	34.0	90a → 91a	---	0.95884
					90a → 92a	---	0.01518
3	2	3	700.1	40.8	88a → 94a	---	0.79230
					87a → 94a	---	0.11738
4	1	1	685.0	41.7	90a → 91a	0.0008022	0.97220
					---	---	---
5	13	3	654.9	43.7	87a → 94a	---	0.76446
					88a → 94a	---	0.09933
6	3	3	647.7	44.1	89a → 91a	---	0.76152
					87a → 91a	---	0.12192
7	8	3	621.1	46.0	88a → 91a	---	0.84342
					87a → 91a	---	0.01896
8	6	3	597.5	47.8	87a → 91a	---	0.80903
					89a → 91a	---	0.09728
9	7	3	561.6	50.9	89a → 94a	---	0.27140
					85a → 94a	---	0.20986
10	5	3	515.1	55.5	88a → 91a	---	0.43424
					90a → 94a	---	0.38209
11	2	1	499.1	57.3	88a → 91a	0.0049816	0.43424
					90a → 94a	---	0.38209
12	10	3	489.4	58.4	90a → 92a	---	0.63866
					85a → 91a	---	0.28025
13	11	3	473.1	60.4	85a → 91a	---	0.56985
					90a → 92a	---	0.32997
14	3	1	471.9	60.6	89a → 91a	0.0019717	0.60213
					88a → 94a	---	0.25483
15	12	3	456.8	62.6	90a → 93a	---	0.97175
					---	---	---
16	9	1	437.6	65.3	90a → 92a	0.0004057	0.93755
					85a → 91a	---	0.02892
17	4	1	436.6	65.5	90a → 94a	0.0042122	0.44811
					87a → 91a	---	0.21201
18	11	1	428.9	66.7	86a → 91a	0.0009630	0.61475
					90a → 93a	---	0.33337
19	5	1	418.4	68.3	88a → 94a	0.0035092	0.61036
					89a → 91a	---	0.28106
20	8	1	414.8	68.9	87a → 91a	0.0473264	0.47012
					88a → 91a	---	0.21114

Table S2B-1. Compound **2** – CASSCF/QD-NEVPT2 lowest transition energies in the gas phase. 5o, 8e Active Space. 10 triplet roots, 10 singlet roots. Orbitals (in order for CI vector notation below): d(z^2), d(xz), d(yz), d(xy), d(x^2-y^2).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
0	0	1	---	---	22220	---	0.9515
					22022	---	0.0127
1	0	3	1175.9	24.3	12221	---	0.9996
					---	---	---
2	1	3	963.0	29.7	22121	---	0.8786
					21221	---	0.0926
3	2	3	891.6	32.1	21221	---	0.8834
					22121	---	0.0919
4	3	3	627.0	45.6	22211	---	0.9394
					21122	---	0.0578
5	1	1	420.7	68.0	12221	0.0000621	0.9806
					20222		0.0088
6	2	1	407.6	70.1	22121	0.0000131	0.9097
					21221		0.0496
7	3	1	391.7	73.0	21221	0.0001101	0.9245
					22121		0.0488
8	4	1	385.2	74.2	22211	0.0000915	0.9826
					22121		0.0155
9	4	3	293.2	97.5	12212	---	0.9890
					22112	---	0.0055
10	5	3	288.5	99.1	22112	---	0.7613
					21212	---	0.0649

Table S2B-2. Compound **2** – CASSCF/QD-NEVPT2 lowest transition energies with CPCM(THF). 5o, 8e Active Space – 10 triplet roots, 10 singlet roots. Orbitals (in order for CI vector notation below): $d(z^2)$, d(xz), d(yz), d(xy), $d(x^2-y^2)$.

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
0	0	1	---	---	22220	---	0.9510
					02222	---	0.0211
1	0	3	1237.6	23.1	12221	---	0.9992
					---	---	---
2	1	3	1011.0	28.3	22121	---	0.9053
					21221	---	0.0672
3	2	3	941.0	30.4	21221	---	0.9075
					22121	---	0.0668
4	3	3	635.5	45.0	22211	---	0.9379
					21122	---	0.0611
5	1	1	426.9	67.0	12221	0.0000485	0.9796
					20222	---	0.0090
6	2	1	414.6	69.0	22121	0.0000040	0.9339
					21221	---	0.0351
7	3	1	399.8	71.5	21221	0.0001066	0.9353
					22121	---	0.0359
8	4	1	387.0	73.9	22211	0.0000935	0.9944
					22121	---	0.0048
9	4	3	297.1	96.2	12212	---	0.9759
					21212	---	0.0145
10	5	3	293.3	97.5	22112	---	0.7716
					11222	---	0.1477

Table S2C-1. Compound **2** – CASSCF/QD-NEVPT2 lowest transition energies in the gas phase. 9o, 10e Active Space – 25 triplet roots, 15 singlet roots. Orbitals (in order for CI vector notation below): bonding $d(x^2-y^2)/C(sp^2)$, d(xy), d(xz), d(yz), $d(z^2)$, $d(x^2-y^2)/C(sp^2)^*$, π*(1), π*(2), π*(3).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
0	0	1	---	---	222220000	---	0.5464
					222120100	---	0.1039
					122221000	---	0.0858
1	0	3	970.1	29.5	222211000	---	0.4539
					122212000	---	0.1696
2	1	3	804.6	35.5	222121000	---	0.6017
					212221000	---	0.1400
3	2	3	758.2	37.7	212221000	---	0.5703
					222121000	---	0.1536
4	3	3	737.1	38.8	222210100	---	0.5396
					122220100	---	0.2880
5	1	1	729.4	39.2	222210100	0.0019683	0.5703
					122220100	---	0.2712
6	4	3	642.1	44.5	222120100	---	0.8142
					122112100	---	0.0417
7	2	1	624.3	45.8	222120100	0.0905865	0.6714
					212220100	---	0.0655
8	5	3	592.5	48.3	221221000	---	0.6680
					212122000	---	0.0822
9	6	3	571.6	50.0	212220100	---	0.7675
					212202100	---	0.0438
10	3	1	569.9	50.2	212220100	0.1206524	0.6956
					112212100	---	0.0370
11	4	1	444.4	64.3	221220100	0.0003508	0.7306
					212121100	---	0.0444
12	7	3	433.9	65.9	222210010	---	0.4812
					122220010	---	0.2506
13	5	1	432.7	66.1	222210010	0.0010716	0.4782
					122220010	---	0.2503
14	8	3	429.9	66.5	221220100	---	0.7217
					212121100	---	0.0699
15	6	1	410.4	69.7	222120010	0.0274877	0.3593
					222211000	---	0.1504
16	7	1	404.5	70.7	222120001	0.0141815	0.2505
					222211000	---	0.1880
17	9	3	400.6	71.4	222120010	---	0.7918
					122112010	---	0.0430
18	8	1	399.8	71.5	222121000	0.0076735	0.4769
					222120010	---	0.0742
19	9	1	396.4	72.1	222210001	0.0025346	0.3590
					122220001	---	0.1937
20	10	3	389.0	73.5	222210001	---	0.5095
					122220001	---	0.2709

Table S2C-2. Compound **2** – CASSCF/QD-NEVPT2 lowest transition energies with CPCM(THF). 9o, 10e Active Space – 25 triplet roots, 15 singlet roots. Orbitals (in order for CI vector notation below): bonding $d(x^2\text{-}y^2)/C(sp^2)$, d(xy), d(xz), d(yz), $d(z^2)$, $d(x^2\text{-}y^2)/C(sp^2)^*$, π*(1), π*(2), π*(3).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
0	0	1	---	---	222220000	---	0.5730
					222120100	---	0.1468
					122221000	---	0.0958
1	0	3	881.1	32.4	222211000	---	0.7022
					122212000	---	0.1274
2	1	3	794.6	36.0	222210100	---	0.7593
					022212100	---	0.0692
3	1	1	768.5	37.2	222210100	0.0013739	0.7523
					022212100	---	0.0686
4	2	3	747.1	38.3	221221000	---	0.4723
					222121000	---	0.2884
5	3	3	698.1	41.0	222121000	---	0.3430
					221221000	---	0.2101
6	4	3	681.7	41.9	222120100	---	0.5581
					222121000	---	0.1158
7	2	1	645.2	44.3	221220100	0.0410929	0.4915
					222120100	---	0.2839
8	5	3	606.9	47.1	221220100	---	0.7427
					222120100	---	0.0615
9	3	1	577.4	49.5	221220100	0.1644325	0.3046
					222120100	---	0.2834
10	6	3	570.0	50.2	212221000	---	0.7017
					221122000	---	0.0669
11	4	1	461.1	62.0	212220100	0.0001703	0.7321
					221121100	---	0.0719
12	7	3	451.1	63.4	222210010	---	0.3902
					212220100	---	0.3515
13	8	3	449.1	63.7	212220100	---	0.4083
					222210010	---	0.3346
14	5	1	448.7	63.7	222210010	0.0030332	0.6533
					222120010	---	0.0760
15	6	1	439.7	65.0	222120010	0.1016451	0.4437
					221220010	---	0.1562
16	9	3	416.2	68.7	222120010	---	0.7280
					22122010	---	0.0705
17	7	1	413.6	69.1	222210001	0.0097205	0.5953
					222211000	---	0.1138
18	10	3	402.8	71.0	222210001	---	0.7274
					022212001	---	0.0661
19	8	1	397.2	72.0	222121000	0.0315108	0.2618
					222120001	---	0.1434
20	9	1	392.8	72.8	222121000	0.0000160	0.2800
					212221000	---	0.2335

Table S2C-3. Compound **2** – CASSCF/QD-NEVPT2 lowest transition energies in gas phase 9o, 10e Active Space – 25 triplet roots, 25 singlet roots. Orbitals (in order for CI vector notation below): d(z^2), d(xz), d(xy), d(yz), bonding d(x^2-y^2)/C(sp^2), d(x^2-y^2)/C(sp^2)*, π*(1), π*(2), π*(3).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
0	0	1	---	---	222220000	---	0.5529
					222211000	---	0.1358
					222120100	---	0.0884
1	0	3	1069.5	26.7	122221000	---	0.4330
					222211000	---	0.2996
2	1	3	814.6	35.1	212221000	---	0.4162
					222121000	---	0.3044
3	2	3	776.5	36.8	222121000	---	0.4340
					212221000	---	0.2879
4	3	3	739.2	38.7	122220100	---	0.4187
					222210100	---	0.3986
5	1	1	731.2	39.1	122220100	0.0032771	0.4253
					222210100	---	0.3978
6	4	3	644.6	44.4	222120100	---	0.8188
					122112100	---	0.0443
7	2	1	634.3	45.1	222120100	0.1012976	0.7104
					222211000	---	0.0384
8	5	3	568.6	50.3	212220100	---	0.4565
					221221000	---	0.2881
9	3	1	565.3	50.6	212220100	0.0896286	0.7351
					212202100	---	0.0675
10	6	3	558.8	51.2	221221000	---	0.3895
					212220100	---	0.3283
11	7	3	471.8	60.6	221220100	---	0.6713
					212121100	---	0.0636
12	8	3	467.7	61.1	122220010	---	0.3885
					222210010	---	0.3303
13	4	1	448.0	63.8	221220100	0.0026610	0.7014
					221202100	---	0.0521
14	5	1	436.5	65.5	122220010	0.0021410	0.3993
					222210010	---	0.3394
15	6	1	421.5	67.8	222120010	0.0471175	0.2936
					122221000	---	0.1924
16	9	3	406.0	70.4	222120010	---	0.7977
					122112010	---	0.0460
17	7	1	398.6	71.7	222121000	0.0012705	0.6168
					122122000	---	0.0491
18	8	1	397.8	71.9	222120010	0.0337901	0.2880
					122221000	---	0.1805
19	10	3	390.3	73.3	122220001	---	0.4339
					222210001	---	0.3609
20	9	1	389.5	73.4	221221000	0.0056080	0.5974
					122220001	---	0.0506

Table S2C-4. Compound **2** – CASSCF/QD-NEVPT2 lowest transition energies with CPCM(THF). 9o, 10e Active Space – 25 triplet roots, 25 singlet roots. Orbitals (in order for CI vector notation below): d(z^2), d(xz), d(xy), d(yz), bonding d(x^2-y^2)/C(sp^2), d(x^2-y^2)/C(sp^2)*, π*(1), π*(2), π*(3).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
0	0	1	---	---	222220000	---	0.5464
					222120100	---	0.1039
					222211000	---	0.0853
1	0	3	970.1	29.5	222211000	---	0.4539
					122221000	---	0.2912
2	1	3	804.6	35.5	222121000	---	0.6017
					212221000	---	0.1400
3	2	3	758.2	37.7	212221000	---	0.5703
					222121000	---	0.1536
4	3	3	737.1	38.8	222210100	---	0.5396
					122220100	---	0.2880
5	1	1	729.4	39.2	222210100	0.0019683	0.5703
					122220100	---	0.2712
6	4	3	642.1	44.5	222120100	---	0.8142
					122112100	---	0.0417
7	2	1	624.3	45.8	222120100	0.0905865	0.6714
					212220100	---	0.0655
8	5	3	592.5	48.3	221221000	---	0.6680
					212122000	---	0.0822
9	6	3	571.6	50.0	212220100	---	0.7675
					112212100	---	0.0416
10	3	1	569.9	50.2	212220100	0.1206524	0.6956
					212202100	---	0.0386
11	4	1	444.4	64.3	221220100	0.0003508	0.7306
					212121100	---	0.0444
12	7	3	433.9	65.9	222210010	---	0.4812
					122220010	---	0.2506
13	5	1	432.7	66.1	222210010	0.0010716	0.4782
					122220010	---	0.2503
14	8	3	429.9	66.5	221220100	---	0.7217
					212121100	---	0.0699
15	6	1	410.4	69.7	222120010	0.0274877	0.3593
					222211000	---	0.1504
16	7	1	404.5	70.7	222120001	0.0141815	0.2505
					222211000	---	0.1880
17	9	3	400.6	71.4	222120010	---	0.7918
					122112010	---	0.0430
18	8	1	399.8	71.5	222120010	0.0076735	0.4769
					222120010	---	0.0742
19	9	1	396.4	72.1	222210001	0.0025346	0.3590
					122220001	---	0.1937
20	10	3	389.0	73.5	222210001	---	0.5095
					122220001	---	0.2709

Table S2D-1. Compound **2** – CASSCF/QD-NEVPT2 composition of the singlet equilibrium ground state in the gas phase. 9o, 10e Active Space – 25 triplet roots, 15 singlet roots. Orbitals: bonding $d(x^2\text{-}y^2)/C(sp^2)$, $d(xy)$, $d(xz)$, $d(yz)$, $d(z^2)$, $d(x^2\text{-}y^2)/C(sp^2)^*$, $\pi^*(1)$, $\pi^*(2)$, $\pi^*(3)$.

CI Vector	Transition	Contribution
222220000	Closed shell singlet (CSS) d^8	0.5509
222120100	$d(yz) \rightarrow \pi^*(1)$	0.1282
122221000	bonding $d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$	0.0888
222210100	$d(z^2) \rightarrow \pi^*(1)$	0.0619
221220001	$d(xz) \rightarrow \pi^*(3)$	0.0363
222120010	$d(yz) \rightarrow \pi^*(2)$	0.0194
222211000	$d(z^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$	0.0142
022122100	$2x[\text{bonding } d(x^2\text{-}y^2)/C(sp^2)] + d(yz) \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*] + \pi^*(1)$	0.0134
221220100	$d(xz) \rightarrow \pi^*(1)$	0.0075
222202000	$2x[d(z^2)] \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*]$	0.0068
022212100	$2x[\text{bonding } d(x^2\text{-}y^2)/C(sp^2)] + d(z^2) \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*] + \pi^*(1)$	0.0067
220222000	$2x[d(xz)] \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*]$	0.0058
122121100	bonding $d(x^2\text{-}y^2)/C(sp^2) + d(yz) + \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$	0.0057
222022000	$2x[d(yz)] \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*]$	0.0057
222210010	$d(z^2) \rightarrow \pi^*(2)$	0.0054
021222001	$2x[\text{bonding } d(x^2\text{-}y^2)/C(sp^2)] + d(xz) \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*] + \pi^*(3)$	0.0031
122112100	bonding $d(x^2\text{-}y^2)/C(sp^2) + d(xz) + d(yz) \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*] + \pi^*(1)$	0.0026
Sum of CSS		55%
Sum of all MLCT		26%
Sum of all d-d		12%
Sum of mixed MLCT + d-d		3.1%

Table S2D-2. Compound **2** – CASSCF/QD-NEVPT2 composition of the singlet equilibrium ground state with CPCM(THF). 9o, 10e Active Space – 25 triplet roots, 15 singlet roots. Orbitals: $d(z^2)$, $d(xz)$, $d(xy)$, $d(yz)$, bonding $d(x^2\text{-}y^2)/C(sp^2)$, $d(x^2\text{-}y^2)/C(sp^2)^*$, $\pi^*(1)$, $\pi^*(2)$, $\pi^*(3)$.

CI Vector	Transition	Contribution
222220000	Closed shell singlet (CSS) d^8	0.5730
222120100	$d(yz) \rightarrow \pi^*(1)$	0.1468
122221000	bonding $d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$	0.0958
221220001	$d(xz) \rightarrow \pi^*(3)$	0.0359
222120010	$d(yz) \rightarrow \pi^*(2)$	0.0206
222210100	$d(z^2) \rightarrow \pi^*(1)$	0.0178
222211000	$d(z^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$	0.0160
022122100	$2x[\text{bonding } d(x^2\text{-}y^2)/C(sp^2)] + d(yz) \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*] + \pi^*(1)$	0.0155
221220100	$d(xz) \rightarrow \pi^*(1)$	0.0119
222202000	$2x[d(z^2)] \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*]$	0.0079
122121100	bonding $d(x^2\text{-}y^2)/C(sp^2) + d(yz) + \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$	0.0066
220222000	$2x[d(xz)] \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*]$	0.0063
222022000	$2x[d(yz)] \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*]$	0.0059
021222001	$2x[\text{bonding } d(x^2\text{-}y^2)/C(sp^2)] + d(xz) \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*] + \pi^*(3)$	0.0030
122112100	bonding $d(x^2\text{-}y^2)/C(sp^2) + d(yz) + d(z^2) \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*] + \pi^*(1)$	0.0025
Sum of CSS		57%
Sum of all MLCT		23%
Sum of all d-d		13%
Sum of mixed MLCT + d-d		2.8%

Table S2D-3. Compound **2** – CASSCF/QD-NEVPT2 composition of the singlet equilibrium ground state in gas phase. 9o, 10e Active Space – 25 triplet roots, 25 singlet roots. Orbitals: $d(z^2)$, d(xz), d(xy), d(yz), bonding $d(x^2\text{-}y^2)/C(sp^2)$, $d(x^2\text{-}y^2)/C(sp^2)^*$, $\pi^*(1)$, $\pi^*(2)$, $\pi^*(3)$.

CI Vector	Transition	Contribution
222220000	Closed shell singlet (CSS) d^8	0.5529
222211000	bonding $d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$	0.1358
222120100	$d(yz) \rightarrow \pi^*(1)$	0.0884
122221000	$d(z^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$	0.0547
212220100	$d(xz) \rightarrow \pi^*(1)$	0.0274
222120010	$d(yz) \rightarrow \pi^*(2)$	0.0265
212220001	$d(xz) \rightarrow \pi^*(3)$	0.0246
122212000	$d(z^2)$ + bonding $d(x^2\text{-}y^2)/C(sp^2) \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*]$	0.0122
202222000	$2x[d(xz)] \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*]$	0.0070
222022000	$2x[d(yz)] \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*]$	0.0069
222102100	$d(yz) + 2x[\text{bonding } d(x^2\text{-}y^2)/C(sp^2)] \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*] + \pi^*(1)$	0.0058
122220100	$d(z^2) \rightarrow \pi^*(1)$	0.0056
122112100	$d(z^2) + d(yz) + \text{bonding } d(x^2\text{-}y^2)/C(sp^2) \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*] + \pi^*(1)$	0.0052
222120001	$d(yz) \rightarrow \pi^*(3)$	0.0051
222210100	bonding $d(x^2\text{-}y^2)/C(sp^2) \rightarrow \pi^*(1)$	0.0039
022222000	$2x[d(z^2)] \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*]$	0.0025
Sum of CSS		55%
Sum of all MLCT		18%
Sum of all d-d		21%
Sum of mixed MLCT + d-d		2.3%

Table S2D-4. Compound **2** – CASSCF/QD-NEVPT2 composition of the singlet equilibrium ground state with CPCM(THF). 9o, 10e Active Space – 25 triplet roots, 25 singlet roots. Orbitals: $d(z^2)$, d(xz), d(xy), d(yz), bonding $d(x^2\text{-}y^2)/C(sp^2)$, $d(x^2\text{-}y^2)/C(sp^2)^*$, $\pi^*(1)$, $\pi^*(2)$, $\pi^*(3)$.

CI Vector	Transition	Contribution
222220000	Closed shell singlet (CSS) d^8	0.5464
222120100	$d(yz) \rightarrow \pi^*(1)$	0.1039
122221000	$d(z^2) \rightarrow d(x^2\text{-}y^2)$	0.0858
222211000	bonding $d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$	0.0853
212220100	$d(xz) \rightarrow \pi^*(1)$	0.0373
212220001	$d(xz) \rightarrow \pi^*(3)$	0.0290
222120010	$d(yz) \rightarrow \pi^*(2)$	0.0236
122212000	$d(z^2)$ + bonding $d(x^2\text{-}y^2)/C(sp^2) \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*]$	0.0122
202222000	$2x[d(xz)] \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*]$	0.0069
222022000	$2x[d(yz)] \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*]$	0.0066
122112100	$d(z^2) + d(yz) + \text{bonding } d(x^2\text{-}y^2)/C(sp^2) \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*] + \pi^*(1)$	0.0063
222120001	$d(yz) \rightarrow \pi^*(3)$	0.0056
022122100	$d(z^2) + d(yz) \rightarrow d(x^2\text{-}y^2) + \pi^*(1)$	0.0054
222210100	bonding $d(x^2\text{-}y^2)/C(sp^2) \rightarrow \pi^*(1)$	0.0053
222102100	$d(yz) + \text{bonding } d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$	0.0030
Sum of CSS		55%
Sum of all MLCT		20%
Sum of all d-d		20%
Sum of mixed MLCT + d-d		1.5%

Table S2E-1. Compound **2** – CASSCF/QD-NEVPT2 lowest transition energies in the gas phase. 10o, 12e Active Space – 20 triplet roots, 10 singlet roots. Orbitals (in order for CI vector notation below): bonding d(xy)/C(π), bonding d(x^2-y^2)/C(sp^2), d(xz), d(xy), d(yz), d(z^2), d(x^2-y^2)/C(sp^2)*, π*(1), π*(2), π*(3).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
0	0	1	---	---	2222220000	---	0.6318
					2222120100	---	0.1391
					2122221000	---	0.0531
1	0	3	1000.6	28.6	2222210100	---	0.8429
					2022212100	---	0.0675
2	1	1	960.9	29.8	2222210100	0.0021210	0.8218
					2022212100		0.0667
3	1	3	846.1	33.8	2222120100	---	0.7748
					2022122100	---	0.0698
4	2	1	775.8	36.9	2212220100	0.0192175	0.5127
					2222120100		0.2761
5	2	3	738.0	38.7	2212220100	---	0.7239
					2012222100	---	0.0538
6	3	3	714.1	40.0	2222211000	---	0.7712
					2122212000	---	0.0802
7	4	3	626.0	45.7	2212221000	---	0.5501
					2222121000	---	0.2572
8	3	1	619.0	46.2	2222120100	0.2167547	0.3590
					2212220100		0.2585
9	5	3	577.6	49.5	2222121000	---	0.5793
					2212221000	---	0.2374
10	4	1	560.2	51.0	2221220100	0.0023581	0.7622
					2212121100		0.0553
11	6	3	541.8	52.8	2221220100	---	0.7308
					2212121100	---	0.0550
12	7	3	524.8	54.5	2221221000	---	0.6806
					2221121100	---	0.0483
13	8	3	455.1	62.8	2222210010	---	0.4270
					2222210001	---	0.4167
14	5	1	433.8	65.9	2222210010	0.0146952	0.7914
					2022212010		0.0650
15	9	3	432.4	66.1	2222210001	---	0.4282
					2222210010	---	0.4100
16	10	3	405.7	70.5	2222120010	---	0.5858
					2212220010	---	0.1251
17	6	1	391.2	73.1	2221221000	0.0017318	0.6850
					2222211000		0.0873
18	7	1	373.8	76.5	2222211000	0.0037102	0.7321
					2221221000		0.0891
19	8	1	364.5	78.4	2222121000	0.0007688	0.4732
					2212221000		0.3645
20	11	3	357.3	80.0	2212220010	---	0.4398
					2222120001	---	0.1767

Table S2E-2. Compound **2** – CASSCF/QD-NEVPT2 lowest transition energies in the gas phase. 10o, 12e Active Space – 25 triplet roots, 15 singlet roots. Orbitals (in order for CI vector notation below): bonding d(xy)/C(π), bonding d(x^2-y^2)/C(sp^2), d(xy), d(xz), d(yz), d(z^2), d(x^2-y^2)/C(sp^2)*, π*(1), π*(2), π*(3).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
0	0	1	---	---	2222220000	---	0.5796
					2222120100	---	0.1775
					2122221000	---	0.0644
1	0	3	922.3	31.0	2222210100	---	0.8168
					2022212100	---	0.0659
2	1	1	890.7	32.1	2222210100	0.00179	0.7846
					2022212100	---	0.0631
3	1	3	809.4	35.3	2222211000	---	0.4160
					2222120100	---	0.3302
4	2	3	778.7	36.7	2222120100	---	0.4159
					2222211000	---	0.3457
5	2	1	720.5	39.7	2221220100	0.03340	0.5256
					2222120100	---	0.2310
6	3	3	686.7	41.6	2221221000	---	0.4526
					2222121000	---	0.3029
7	4	3	675.3	42.3	2221220100	---	0.7063
					2021222100	---	0.0498
8	5	3	638.2	44.8	2222121000	---	0.4856
					2221221000	---	0.3037
9	3	1	632.0	45.2	2222120100	0.17525	0.3036
					2221220100	---	0.2534
10	6	3	549.5	52.0	2212221000	---	0.6054
					2212121100	---	0.0685
11	4	1	517.8	55.2	2212220100	0.00051	0.7254
					2221121100	---	0.0611
12	7	3	509.9	56.1	2212220100	---	0.7244
					2221121100	---	0.0600
13	8	3	489.3	58.4	2222210010	---	0.7691
					2022212010	---	0.0670
14	5	1	487.5	58.6	2222210010	0.00192	0.7185
					2022212010	---	0.0627
15	6	1	458.8	62.3	2222120010	0.09519	0.4058
					2221220010	---	0.1885
16	9	3	452.2	63.2	2222120010	---	0.7398
					2022122010	---	0.0698
17	7	1	442.8	64.6	2222210001	0.01268	0.7254
					2022212001	---	0.0617
18	10	3	430.1	66.5	2222210001	---	0.7692
					2022212001	---	0.0651
19	8	1	430.0	66.5	2221220010	0.00571	0.5576
					2222120010	---	0.1065
20	11	3	409.9	69.7	2221220010	---	0.6892
					2221220001	---	0.0620

Table S2E-3. Compound **2** – CASSCF/QD-NEVPT2 Lowest transition energies with CPCM(THF). 10o, 12e Active Space – 25 triplet roots, 15 singlet roots. Orbitals (in order for CI vector notation below): bonding d(xy)/C(π), bonding $d(x^2-y^2)/C(sp^2)$, d(xy), d(xz), d(yz), $d(z^2)$, $d(x^2-y^2)/C(sp^2)$*, π*(1), π*(2), π*(3).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
0	0	1	---	---	2222220000	---	0.6012
					2222120100	---	0.1574
					2122221000	---	0.0715
1	0	3	907.8	31.5	2222210100	---	0.7864
					2022212100	---	0.0647
2	1	3	816.4	35.0	2222211000	---	0.7763
					2122212000	---	0.0980
3	1	1	805.7	35.5	2222210100	0.0015632	0.7932
					2022212100	---	0.0651
4	2	3	717.2	39.9	2222120100	---	0.7553
					2022122100	---	0.0679
5	2	1	666.5	42.9	2221220100	0.0318143	0.5075
					2222120100	---	0.2601
6	3	3	656.2	43.6	2222121000	---	0.3972
					2221221000	---	0.3808
7	4	3	652.4	43.8	2222121000	---	0.4020
					2221221000	---	0.3910
8	5	3	633.5	45.1	2221220100	---	0.7386
					2222120100	---	0.0451
9	3	1	584.7	48.9	2222120100	0.1984600	0.3109
					2221220100	---	0.2682
10	6	3	547.0	52.3	2212221000	---	0.6240
					2221122000	---	0.0672
11	4	1	487.9	58.6	2212220100	0.0005989	0.7323
					2221121100	---	0.0615
12	7	3	477.5	59.9	2212220100	---	0.7351
					2221121100	---	0.0610
13	8	3	460.5	62.1	2222210010	---	0.6676
					2222210001	---	0.1412
14	5	1	456.2	62.7	2222210010	0.0029045	0.7120
					2022212010	---	0.0633
15	6	1	443.5	64.5	2222120010	0.1027144	0.4285
					2221220010	---	0.1113
16	9	3	429.7	66.5	2222210001	---	0.6684
					2222210010	---	0.1350
17	10	3	424.1	67.4	2222120010	---	0.7429
					2122121010	---	0.0501
18	7	1	410.1	69.7	2222210001	0.0097454	0.6190
					2222211000	---	0.0582
19	8	1	398.6	71.7	2212221000	0.0169288	0.3458
					2222210001	---	0.1354
20	11	3	391.6	73.0	2221220010	---	0.7063
					2221220001	---	0.0557

Table S2E-4. Compound **2** – CASSCF/QD-NEVPT2 lowest transition energies in the gas phase. 10o, 12e Active Space – 40 triplet roots, 25 singlet roots. Orbitals (in order for CI vector notation below): bonding d(xy)/C(π), bonding d(x^2-y^2)/C(sp^2), d(xz), d(yz), d(z^2), d(xy), d(x^2-y^2)/C(sp^2)*, π*(1), π*(2), π*(3).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
0	0	1	---	---	2222220000	---	0.6252
					2221220100	---	0.0660
					2212220100	---	0.0637
1	0	3	846.7	33.8	2222121000	---	0.5072
					2122221000	---	0.1444
2	1	3	791.3	36.1	2222120100	---	0.5010
					2222210100	---	0.1672
3	1	1	770.4	37.1	2222120100	0.0024769	0.5080
					2222210100	---	0.1611
4	2	3	754.4	37.9	2221221000	---	0.7900
					2121222000	---	0.0728
5	3	3	706.9	40.4	2212221000	---	0.6698
					2122221000	---	0.0929
6	4	3	691.6	41.3	2221220100	---	0.7037
					2212220100	---	0.0610
7	2	1	660.5	43.3	2221220100	0.0915113	0.6732
					2222220000	---	0.0387
8	5	3	622.2	46.0	2212220100	---	0.6105
					2122220100	---	0.0586
9	3	1	598.3	47.8	2212220100	0.0987239	0.5993
					2122220100	---	0.0634
10	6	3	573.0	49.9	2222211000	---	0.4666
					2222121000	---	0.1321
11	4	1	476.0	60.1	2222210100	0.0009262	0.4903
					2222120100	---	0.2030
12	7	3	473.2	60.4	2222210100	---	0.5038
					2222120100	---	0.2033
13	8	3	456.7	62.6	2222120010	---	0.4563
					2222210010	---	0.1511
14	5	1	454.8	62.9	2222120010	0.0020837	0.4470
					2222210010	---	0.1435
15	6	1	428.3	66.8	2221220010	0.0399342	0.4974
					2221220001	---	0.2063
16	9	3	424.5	67.4	2221220010	---	0.6741
					2212220010	---	0.0759
17	7	1	407.4	70.2	2222120001	0.0152654	0.4264
					2122220001	---	0.1124
18	10	3	403.2	70.9	2222120001	---	0.4598
					2222210001	---	0.1477
19	8	1	399.7	71.5	2221220001	0.1277239	0.2755
					2212220001	---	0.1806
20	9	1	395.7	72.3	2221221000	0.0091248	0.3478
					2212220010	---	0.1772

Table S2F-1. Compound **2** – CASSCF/QD-NEVPT2 composition of the singlet equilibrium ground state in the gas phase. 10o, 12e Active Space – 20 triplet roots, 10 singlet roots. Orbitals: bonding d(xy)/C(π), bonding d(x^2-y^2)/C(sp^2), d(xz), d(xy), d(yz), d(z^2), d(x^2-y^2)/C(sp^2)*, π*(1), π*(2), π*(3).

CI Vector	Transition	Contribution
2222220000	Closed shell singlet (CSS) d^8	0.6318
2222120100	d(yz) → π*(1)	0.1391
2122221000	bonding d(x^2-y^2)/C(sp^2) → d(x^2-y^2)/C(sp^2)*	0.0531
2212220100	d(xz) → π*(1)	0.0283
2222120001	d(yz) → π*(3)	0.0237
2022122100	2x[bonding d(x^2-y^2)/C(sp^2)] + d(yz)→ 2x[d(x^2-y^2)/C(sp^2)*] + π*(1)	0.0149
2122121100	bonding d(x^2-y^2)/C(sp^2) + d(yz) → d(x^2-y^2)/C(sp^2)* + π*(1)	0.0142
2212220010	d(xz) → π*(2)	0.0134
2222202000	2x[d(z^2)] → 2x[d(x^2-y^2)/C(sp^2)*]	0.0088
2222210100	d(z^2) → π*(1)	0.0088
2202222000	2x[d(xz)] → 2x[d(x^2-y^2)/C(sp^2)*]	0.0055
2222022000	2x[d(yz)] → 2x[d(x^2-y^2)/C(sp^2)*]	0.0050
2122121001	bonding d(x^2-y^2)/C(sp^2) + d(yz) + → d(x^2-y^2)/C(sp^2)* + π*(3)	0.0045
2022122001	2x[bonding d(x^2-y^2)/C(sp^2)] + d(yz)→ 2x[d(x^2-y^2)/C(sp^2)*] + π*(3)	0.0036
2222120010	d(yz) → π*(2)	0.0031
2222111100	d(yz) + d(z^2) → d(x^2-y^2)/C(sp^2)* + π*(1)	0.0029
2112221100	bonding d(x^2-y^2)/C(sp^2) + d(xz) → d(x^2-y^2)/C(sp^2)* + π*(1)	0.0028
2012222100	2x[bonding d(x^2-y^2)/C(sp^2)] + d(xz)→ 2x[d(x^2-y^2)/C(sp^2)*] + π*(1)	0.0027
Sum of CSS		**63%**
Sum of all MLCT		**22%**
Sum of all d-d		**7.2%**
Sum of mixed MLCT + d-d		**4.6%**

Table S2F-2. Compound **2** – CASSCF/QD-NEVPT2 composition of the singlet equilibrium ground state in the gas phase. 10o, 12e Active Space – 25 triplet roots, 15 singlet roots. Orbitals: bonding d(xy)/C(π), bonding $d(x^2\text{-}y^2)/C(sp^2)$, d(xy), d(xz), d(yz), $d(z^2)$, $d(x^2\text{-}y^2)/C(sp^2)$*, π*(1), π*(2), π*(3).

CI Vector	Transition	Contribution
2222220000	Closed shell singlet (CSS) d^8	0.5796
2222120100	d(yz) → π*(1)	0.1775
2122221000	bonding $d(x^2\text{-}y^2)/C(sp^2)$ → $d(x^2\text{-}y^2)/C(sp^2)$*	0.0644
2222120010	d(yz) → π*(2)	0.0235
2221220001	d(xz) → π*(3)	0.0218
2022122100	2x[bonding $d(x^2\text{-}y^2)/C(sp^2)$] + d(yz) → 2x[$d(x^2\text{-}y^2)/C(sp^2)$*] + π*(1)	0.0174
2222210100	$d(z^2)$ → π*(1)	0.0143
2221220100	d(xz) → π*(1)	0.0121
2122121100	bonding $d(x^2\text{-}y^2)/C(sp^2)$ + d(yz) → $d(x^2\text{-}y^2)/C(sp^2)$* + π*(1)	0.0121
2222202000	2x[$d(z^2)$] → 2x[$d(x^2\text{-}y^2)/C(sp^2)$*]	0.0083
2222211000	$d(z^2)$ → $d(x^2\text{-}y^2)/C(sp^2)$*	0.0079
2220222000	2x[d(xz)] → 2x[$d(x^2\text{-}y^2)/C(sp^2)$*]	0.0056
2222022000	2x[d(yz)] → 2x[$d(x^2\text{-}y^2)/C(sp^2)$*]	0.0052
2222111100	d(yz) + $d(z^2)$ → $d(x^2\text{-}y^2)/C(sp^2)$* + π*(1)	0.0031
2212221000	d(xy) → $d(x^2\text{-}y^2)/C(sp^2)$*	0.0029
2022122010	2x[bonding $d(x^2\text{-}y^2)/C(sp^2)$] + d(yz) → $d(x^2\text{-}y^2)/C(sp^2)$* + π*(2)	0.0025
Sum of CSS		**58%**
Sum of all MLCT		**25%**
Sum of all d-d		**9.4%**
Sum of mixed MLCT + d-d		**3.5%**

Table S2F-3. Compound **2** – CASSCF/QD-NEVPT2 composition of the singlet equilibrium ground state with CPCM(THF). 10o, 12e Active Space – 25 triplet roots, 15 singlet roots. Orbitals: bonding d(xy)/C(π), bonding $d(x^2\text{-}y^2)/C(sp^2)$, d(xy), d(xz), d(yz), $d(z^2)$, $d(x^2\text{-}y^2)/C(sp^2)$*, π*(1), π*(2), π*(3).

CI Vector	Transition	Contribution
2222220000	Closed shell singlet (CSS) d^8	0.6012
2222120100	d(yz) → π*(1)	0.1574
2122221000	bonding $d(x^2\text{-}y^2)/C(sp^2)$ → $d(x^2\text{-}y^2)/C(sp^2)$*	0.0715
2222120010	d(yz) → π*(2)	0.0222
2221220001	d(xz) → π*(3)	0.0195
2022122100	d(xz) → π*(1)	0.0165
2222210100	2x[bonding $d(x^2\text{-}y^2)/C(sp^2)$] + d(yz) → 2x[$d(x^2\text{-}y^2)/C(sp^2)$*] + π*(1)	0.0157
2221220100	bonding $d(x^2\text{-}y^2)/C(sp^2)$ + d(yz) → $d(x^2\text{-}y^2)/C(sp^2)$* + π*(1)	0.0112
2122121100	$d(z^2)$ → π*(1)	0.0099
2222202000	2x[$d(z^2)$] → 2x[$d(x^2\text{-}y^2)/C(sp^2)$*]	0.0090
2222211000	$d(z^2)$ → $d(x^2\text{-}y^2)/C(sp^2)$*	0.0085
2220222000	2x[d(xz)] → 2x[$d(x^2\text{-}y^2)/C(sp^2)$*]	0.0062
2222022000	2x[d(yz)] → 2x[$d(x^2\text{-}y^2)/C(sp^2)$*]	0.0057
2222111100	d(yz) + $d(z^2)$ → $d(x^2\text{-}y^2)/C(sp^2)$* + π*(1)	0.0028
Sum of CSS		**60%**
Sum of all MLCT		**23%**
Sum of all d-d		**10%**
Sum of mixed MLCT + d-d		**3.0%**

Table S2F-4. Compound **2** – CASSCF/QD-NEVPT2 composition of the singlet equilibrium ground state in the gas phase. 10o, 12e Active Space – 40 triplet roots, 25 singlet roots. Orbitals: bonding d(xy)/C(π), bonding $d(x^2\text{-}y^2)/C(sp^2)$, d(xz), d(yz), $d(z^2)$, d(xy), $d(x^2\text{-}y^2)/C(sp^2)$*, π*(1), π*(2), π*(3).

CI Vector	Transition	Contribution
2222220000	Closed shell singlet (CSS) d^8	0.6252
2221220100	d(yz) → π*(1)	0.0660
2212220100	d(xz) → π*(1)	0.0637
2122221000	bonding $d(x^2\text{-}y^2)/C(sp^2)$ → $d(x^2\text{-}y^2)/C(sp^2)$*	0.0441
2212220001	d(xz) → π*(3)	0.0200
2221220010	d(yz) → π*(2)	0.0188
2222121000	$d(z^2)$ → $d(x^2\text{-}y^2)/C(sp^2)$*	0.0150
2221220001	d(yz) → π*(3)	0.0127
2222211000	d(xy) → $d(x^2\text{-}y^2)/C(sp^2)$*	0.0104
2122220100	bonding $d(x^2\text{-}y^2)/C(sp^2)$* → π*(1)	0.0098
2212220010	d(xz) → π*(2)	0.0077
2220222000	2x[d(yz)] → 2x[$d(x^2\text{-}y^2)/C(sp^2)$*]	0.0061
2221121100	d(yz) + $d(z^2)$ → $d(x^2\text{-}y^2)/C(sp^2)$* + π*(1)	0.0055
2202222000	2x[d(xz)] → 2x[$d(x^2\text{-}y^2)/C(sp^2)$*]	0.0055
2222022000	2x[$d(z^2)$] → 2x[$d(x^2\text{-}y^2)/C(sp^2)$*]	0.0047
2122220001	bonding $d(x^2\text{-}y^2)/C(sp^2)$ → π*(3)	0.0046
2021222100	2x[bonding $d(x^2\text{-}y^2)/C(sp^2)$] + d(yz) → 2x[$d(x^2\text{-}y^2)/C(sp^2)$*] + π*(1)	0.0045
2212221000	d(xz) → $d(x^2\text{-}y^2)/C(sp^2)$*	0.0041
2012222100	2x[bonding $d(x^2\text{-}y^2)/C(sp^2)$] + d(xz) → 2x[$d(x^2\text{-}y^2)/C(sp^2)$*] + π*(1)	0.0036
2121221100	bonding $d(x^2\text{-}y^2)/C(sp^2)$ + d(yz) → $d(x^2\text{-}y^2)/C(sp^2)$* + π*(1)	0.0034
2222120100	$d(z^2)$ → π*(1)	0.0032
2112221100	bonding $d(x^2\text{-}y^2)/C(sp^2)$ + d(xz) → $d(x^2\text{-}y^2)/C(sp^2)$* + π*(1)	0.0030
2222210100	d(xy) → π*(1)	0.0026
1222221000	bonding d(xy)/C(π) → $d(x^2\text{-}y^2)/C(sp^2)$*	0.0026
Sum of CSS		**63%**
Sum of all MLCT		**21%**
Sum of all d-d		**9.3%**
Sum of mixed MLCT + d-d		**2.0%**

Table S2G. Compound **2** –CASSCF/QD-NEVPT2 composition of the singlet equilibrium ground state while varying number roots. 9o, 10e Active Space – 25 triplet roots, *X* singlet roots (where *X* ranged from 15 to 25). Orbitals: bonding $d(x^2\text{-}y^2)/C(sp^2)$, d(xy), d(xz), d(yz), $d(z^2)$, $d(x^2\text{-}y^2)/C(sp^2)^*$, π*(1), π*(2), π*(3). 10o, 12e Active Space – *X* triplet roots, *Y* singlet roots where *X* ranged from 20 to 40, and *Y* ranged from 10 to 25. Orbitals: bonding d(xy)/C(π), bonding $d(x^2\text{-}y^2)/C(sp^2)$, d(xy), d(xz), d(yz), $d(z^2)$, $d(x^2\text{-}y^2)/C(sp^2)^*$, π*(1), π*(2), π*(3).

Weights of Three Most Dominant Terms in CI-Vector (# Triplets / # Singlets)

Active Spaces:	9 orbitals, 10 electrons				10 orbitals, 12 electrons			
Configuration	**25/15 Gas**	**25/15 CPCM**	**25/25 Gas**	**25/25 CPCM**	**20/10 Gas**	**25/15 Gas**	**25/15 CPCM**	**40/25 Gas**
CSS	0.5509	0.5730	0.5529	0.5464	0.6318	0.5796	0.6012	0.6252
$d(yz) \rightarrow \pi^*(1)$	0.1282	0.1468	0.0884	0.1039	0.1391	0.1775	0.1574	0.0660[†]
$d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$	0.0888	0.0958	0.1358	0.0853[‡]	0.0531	0.0644	0.0715	0.0441

Sums of Weights

Active Spaces:	9 orbitals, 10 electrons				10 orbitals, 12 electrons			
Configuration	**25/15 Gas**	**25/15 CPCM**	**25/25 Gas**	**25/25 CPCM**	**20/10 Gas**	**25/15 Gas**	**25/15 CPCM**	**40/25 Gas**
CSS	55%	57%	55%	55%	63%	58%	60%	63%
Sum of MLCT	26%	23%	18%	20%	22%	25%	23%	21%
Sum of d-d	12%	13%	21%	20%	7.2%	9.4%	10%	9.3%
Sum of MLCT+d-d	3.1%	2.8%	2.3%	1.5%	4.6%	3.5%	3.0%	2.0%

Singlet → Singlet Transition Energies (kcal mol^{-1})

Active Spaces:	9 orbitals, 10 electrons				10 orbitals, 12 electrons			
Transition	**25/15 Gas**	**25/15 CPCM**	**25/25 Gas**	**25/25 CPCM**	**20/10 Gas**	**25/15 Gas**	**25/15 CPCM**	**40/25 Gas**
$S_0 \rightarrow S_1$	33.3	37.2	39.1	39.2	29.8	32.1	35.5	37.1
$S_0 \rightarrow S_2$	40.6	44.3	45.1	45.8	36.9	39.7	42.9	43.3
$S_0 \rightarrow S_3$	45.5	49.5	50.6	50.2	46.2	45.2	48.9	47.8
$S_0 \rightarrow S_4$	58.1	62.0	63.8	64.3	51.0	55.2	58.6	60.1
$S_0 \rightarrow S_5$	59.3	63.7	65.5	66.1	65.9	58.6	62.7	62.9
$S_0 \rightarrow S_6$	63.7	65.0	67.8	69.7	73.1	62.3	64.5	66.8
$S_0 \rightarrow S_7$	66.3	69.1	71.7	70.7	76.5	64.6	69.7	70.2
$S_0 \rightarrow S_8$	68.2	72.0	71.9	71.5	78.4	66.5	71.7	71.5
$S_0 \rightarrow S_9$	69.2	72.8	73.4	72.1	81.4	71.4	73.7	72.3
$S_0 \rightarrow S_{10}$	73.0	74.1	73.5	74.3	---	75.5	74.7	72.7
$S_0 \rightarrow S_{11}$	74.6	75.3	75.2	74.8	---	76.9	76.5	74.2
$S_0 \rightarrow S_{12}$	75.9	77.7	77.2	75.7	---	78.7	78.7	76.9
$S_0 \rightarrow S_{13}$	79.0	80.4	79.8	77.5	---	80.2	81.2	77.2
$S_0 \rightarrow S_{14}$	82.6	86.3	84.2	87.1	---	112.7	116.2	84.2

[†] $d(xz) \rightarrow \pi^*(1)$ is 0.0637. [‡] $d(z^2) \rightarrow d(x^2\text{-}y^2)$ is slightly higher at 0.0858.

Table S2H-1. Compound **2** with Ni–C distance of 3.14 Å – CASSCF/QD-NEVPT2 lowest transition energies in the gas phase. 8o, 10e Active Space – 25 triplet roots, 15 singlet roots. Orbitals (in order for CI vector notation below): d(xz), d(yz), d(xy), $d(z^2)$, $d(x^2\text{-}y^2)$, $C(sp^2)^*$, π*(1), π*(2).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
0	0	3†	---	---	12221110	---	0.4414
					22211110	---	0.0777
					21221110	---	0.0769
1	0	1†	1.35E+05	0.2	12221110	---	0.4544
					22220110	---	0.1621
2	1	3	11691.9	2.4	22211110	0.0000185	0.5698
					22211200	---	0.1445
3	1	1	6953.1	4.1	22211110	---	0.7473
					21221110	---	0.0745
4	2	3	6042.1	4.7	22211110	0.0000044	0.5075
					21221110	---	0.1900
5	3	3	5510.1	5.2	22211110	0.0000638	0.3270
					21221110	---	0.3178
6	2	1	4415.9	6.5	22220110	---	0.4317
					12221110	---	0.2298
7	4	3	3990.5	7.2	12221110	0.0000214	0.4491
					22220110	---	0.1777
8	5	3	3896.3	7.3	21221110	0.0000363	0.6461
					22220110	---	0.1142
9	3	1	3858.7	7.4	21221110	---	0.7457
					12221110	---	0.0583
10	6	3	3537.3	8.1	22220110	0.0000600	0.4848
					12221110	---	0.2458
11	7	3	1142.4	25.0	22121110	0.0000216	0.4116
					22121200	---	0.1173
12	4	1	1063.8	26.9	22121110	---	0.5493
					11222110	---	0.2679
13	8	3	1042.4	27.4	22121110	0.0000031	0.5686
					11222110	---	0.2627
14	9	3	966.1	29.6	21221101	0.0536947	0.4585
					12221101	---	0.1746
15	5	1	953.6	30.0	22211101	---	0.4312
					21221101	---	0.2753
16	10	3	947.7	30.2	22211101	0.0008840	0.7957
					22211011	---	0.0538
17	6	1	916.4	31.2	22211101	---	0.3968
					21221101	---	0.2779
18	11	3	887.2	32.2	22211101	0.0003050	0.7210
					21221101	---	0.1448
19	12	3	847.2	33.7	21221101	0.0000199	0.8183
					21221011	---	0.0548
20	13	3	825.5	34.6	12221101	0.0035754	0.7783
					22121101	---	0.0461

†The lowest singlet and triplet roots are essentially isoenergetic.

Table S2H-2. Compound **2** with Ni–C distance of 3.14 Å – CASSCF/QD-NEVPT2 lowest transition energies with CPCM(THF). 8o,10e Active Space – 25 triplet roots, 15 singlet roots. Orbitals (in order for CI vector notation below): d(xy), d(xz), d(z^2), d(yz), d(x^2-y^2), C(sp^2)*, π*(1), π*(2).

State	Root	Multiplicity	ΔE/nm	ΔE/kcal mol^{-1}	CI Vector	f_{osc}	Contribution
0	0	3†	---	---	21221110	---	0.4372
					22121110	---	0.1725
					22211110	---	0.0831
1	0	1†	5.9E+04	0.5	21221110	---	0.4877
					22220110	---	0.1626
2	1	3	13662.2	2.1	22121110	0.0000327	0.5328
					22211110	---	0.1036
3	1	1	7957.3	3.6	22121110	---	0.8617
					21221110	---	0.0331
4	2	3	6570.1	4.4	22121110	0.0000085	0.6242
					22211110	---	0.1966
5	3	3	5735.6	5.0	22211110	0.0000302	0.3595
					22121110	---	0.2485
6	2	1	4184.7	6.8	22220110	---	0.5189
					21221110	---	0.1758
7	4	3	4034.3	7.1	21221110	0.0000046	0.6509
					22220110	---	0.0728
8	5	3	3982.8	7.2	22211110	0.0000565	0.7504
					21221110	---	0.0852
9	3	1	3963.4	7.2	22211110	---	0.7430
					21221110	---	0.1371
10	6	3	3416.6	8.4	22220110	0.0000134	0.7020
					21221110	---	0.1408
11	7	3	1144.3	25.0	12221110	0.0000176	0.5107
					21212110	---	0.2185
12	4	1	1068.5	26.8	12221110	---	0.6071
					21212110	---	0.2776
13	8	3	1043.9	27.4	12221110	0.0000045	0.6244
					21212110	---	0.2658
14	5	1	1007.8	28.4	22121101	---	0.7969
					21221101	---	0.0324
15	9	3	989.2	28.9	22121101	0.0042687	0.6679
					22211101	---	0.1223
16	10	3	975.5	29.3	22121101	0.0457152	0.4067
					22211101	---	0.3207
17	6	1	953.3	30.0	22211101	---	0.6362
					21221101	---	0.1400
18	11	3	925.9	30.9	22121101	0.0001487	0.6010
					22211101	---	0.3172
19	12	3	883.5	32.4	22211101	0.0000838	0.8077
					21122101	---	0.0425
20	7	1	862.1	33.2	21221101	---	0.6712
					22211101		0.1758

†The lowest singlet and triplet roots are essentially isoenergetic.

Table S2I-1. Compound **2** – CASSCF/QD-NEVPT2 composition with Ni–C distance of 3.14 Å – CASSCF/QD-NEVPT2 composition of the lowest singlet root in the gas phase. 8o, 10e Active Space – 25 triplet roots, 15 singlet roots. Orbitals (in order for CI vector notation below): d(xz), d(yz), d(xy), d(z^2), d(x^2-y^2), C(sp^2)*, π*(1), π*(2).

CI Vector	Transition	Contribution
12221110	d(xz) + d(x^2-y^2) → C(sp^2)* + π*(1)	0.4544
22220110	2x[d(x^2-y^2)] → C(sp^2)* + π*(1)	0.1621
22211110	d(z^2) + d(x^2-y^2) → C(sp^2)* + π*(1)	0.0698
22220200	2x[d(x^2-y^2)] → 2x[C(sp^2)*]	0.0422
21221110	d(yz) + d(x^2-y^2) → C(sp^2)* + π*(1)	0.0279
22220020	2x[d(x^2-y^2)] → 2x[π*(1)]	0.0270
12222010	d(xz) → π*(1)	0.0157
21122110	d(yz) + d(xy) → C(sp^2)* + π*(1)	0.0151
21221101	d(yz) + d(x^2-y^2) → C(sp^2)* + π*(2)	0.0149
21212110	d(yz) + d(z^2) → C(sp^2)* + π*(1)	0.0144
22121110	d(xy) + d(x^2-y^2) → C(sp^2)* + π*(2)	0.0105
12220210	d(xz) + 2x[d(x^2-y^2)] → 2x[C(sp^2)*] + π*(1)	0.0092
12222100	d(xz) → C(sp^2)*	0.0067
12221101	d(xz) + d(x^2-y^2) → C(sp^2)* + π*(2)	0.0065
22202110	2x[d(z^2)] → C(sp^2)* + π*(1)	0.0056
20222110	2x[d(yz)] → C(sp^2)* + π*(1)	0.0039
02222110	2x[d(xz)] → C(sp^2)* + π*(1)	0.0038

Table S2I-2. Compound **2** – CASSCF/QD-NEVPT2 composition with Ni–C distance of 3.14 Å – CASSCF/QD-NEVPT2 composition of the lowest singlet root with CPCM(THF). 8o, 10e Active Space – 25 triplet roots, 15 singlet roots. Orbitals (in order for CI vector notation below): d(xy), d(xz), d(z^2), d(yz), d(x^2-y^2), C(sp^2)*, π*(1), π*(2).

CI Vector	Transition	Contribution
21221110	d(yz) + d(x^2-y^2) → C(sp^2)* + π*(1)	0.4877
22220110	2x[d(x^2-y^2)] → C(sp^2)* + π*(1)	0.1626
22211110	d(z^2) + d(x^2-y^2) → C(sp^2)* + π*(1)	0.0842
22221100	d(x^2-y^2) → C(sp^2)*	0.0671
22121110	d(xy) + d(x^2-y^2) → C(sp^2)* + π*(1)	0.0307
22220200	2x[d(x^2-y^2)] → 2x[C(sp^2)*]	0.0273
22112110	d(xy) + d(z^2) → C(sp^2)* + π*(1)	0.0189
22220020	2x[d(x^2-y^2)] → 2x[π*(1)]	0.0149
12212110	d(xz) + d(z^2) → C(sp^2)* + π*(1)	0.0136
21222010	d(yz) → π*(1)	0.0123
22211101	d(z^2) + d(x^2-y^2) → C(sp^2)* + π*(2)	0.0102
12221110	d(xz) + d(x^2-y^2) → C(sp^2)* + π*(1)	0.0087
21220210	d(yz) + 2x[d(x^2-y^2)] → 2x[C(sp^2)*] + π*(1)	0.0071
22022110	2x[d(xy)] → C(sp^2)* + π*(1)	0.0064
21222100	d(xz) → C(sp^2)*	0.0060
22121101	d(xy) + d(x^2-y^2) → C(sp^2)* + π*(2)	0.0053
20222110	2x[d(yz)] → C(sp^2)* + π*(1)	0.0044
22202110	2x[d(z^2)] → C(sp^2)* + π*(1)	0.0038
21221101	d(yz) + d(x^2-y^2) → C(sp^2)* + π*(2)	0.0028

Table S2J. Compound **2** – CASSCF/QD-NEVPT2 composition of the formal Ni(I) ground state while varying number of doublet roots. 8o, 9e Active Space – 25 quartet roots, *X* doublet roots (where *X* ranged from 15 to 45).

CI-Vector Weights (# Quartets / # Doublets)					
Transition	**25/15 CPCM**	**25/15 Gas**	**25/25 Gas**	**25/35 Gas**	**25/45 Gas**
d(xz) → π*(1)	0.6210	0.6788	0.6610	0.6567	0.6650
$d(x^2-y^2)$ → π*(1)	0.0887	0.0995	0.1219	0.1153	0.1245
formal Ni(I)	0.0671	0.0691	0.0680	0.0707	0.0693
Doublet→Doublet Transition Energies (kcal mol^{-1})					
Transition	**25/15 CPCM**	**25/15 Gas**	**25/25 Gas**	**25/35 Gas**	**25/45 Gas**
1	5.1	6.1	6.3	6.6	6.6
2	7.4	7.7	7.8	8.0	8.0
3	9.6	9.3	8.6	8.9	8.6
4	26.8	27.0	25.8	26.2	26.3
5	28.8	29.1	29.2	29.4	29.5
6	32.4	33.3	33.7	34.0	34.1
7	35.2	35.6	35.4	35.9	35.6
8	37.0	37.9	35.8	36.2	36.3
9	38.6	39.0	38.2	38.5	38.6
10	41.2	41.3	39.3	39.6	39.6
11	49.7	50.6	39.4	39.8	39.7
12	50.8	51.7	41.6	42.0	42.1
13	55.1	56.1	49.7	49.9	49.9
14	57.3	58.7	50.8	51.1	50.9

Table S2K. Leadings terms of CI-vector for the T_0 (first triplet manifold reached from vertical excitation of singlet ground state) of **2** in Figure S2J. Just past the equilibrium geometry, the CI-vector is dominated by ^{3}d-d transitions. Note that using the relaxed, DFT optimized C_{4v} triplet geometries of **2** (surfaces shown in Figure S2G) the ground state triplet CI-vector is very heavily dominated by the $[d(x^2\text{-}y^2)]^1[d(z^2)/C(sp^2)^*]^1$ ^{3}d-d transition (64% at the 1.95 Å equilibrium geometry, Figure S2I bottom). At long Ni–C distances, the transition d(xz) → π*(1) is becomes dominant, making for a $[d(xz)]^1[d(x^2\text{-}y^2)]^1[(dz^2)/C(sp^2)^*]^1[\pi^*(1)]^1$ configuration.

Ni–C Distance (Å)	Weight	Transition
1.89 (equil.)	0.8168	$d(z^2) \rightarrow \pi^*(1)$
	0.0659	$2x[\text{bonding } d(x^2\text{-}y^2)/C(sp^2)] + d(z^2) \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*] + \pi^*(1)$
2.02	0.4339	$d(z^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$
	0.2551	$\text{bonding } d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$
2.21	0.3666	$\text{bonding } d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$
	0.2786	$d(z^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$
2.40	0.5334	$d(z^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^*$
	0.3130	$d(z^2) + \text{bonding } d(x^2\text{-}y^2)/C(sp^2) \rightarrow 2x[d(x^2\text{-}y^2)/C(sp^2)^*]$
2.60	0.4218	$d(z^2) \rightarrow \pi^*(1)$
	0.3788	$d(z^2) + \text{bonding } d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$
2.91	0.6157	$d(z^2) + \text{bonding } d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$
	0.2267	$d(z^2) \rightarrow \pi^*(1)$
3.14	0.4414	$d(xz) + \text{bonding } d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$
	0.0777	$d(z^2) + \text{bonding } d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$
3.31	0.5253	$d(xz) + \text{bonding } d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$
	0.1070	$2x[\text{bonding } d(x^2\text{-}y^2)/C(sp^2)] \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$
3.49	0.6173	$d(xz) + \text{bonding } d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$
	0.1150	$2x[\text{bonding } d(x^2\text{-}y^2)/C(sp^2)] \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$
3.71	0.2595	$d(yz) + \text{bonding } d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$
	0.1641	$2x[\text{bonding } d(x^2\text{-}y^2)/C(sp^2)] \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$
3.94	0.2298	$d(yz) + \text{bonding } d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$
	0.2117	$d(xz) + \text{bonding } d(x^2\text{-}y^2)/C(sp^2) \rightarrow d(x^2\text{-}y^2)/C(sp^2)^* + \pi^*(1)$

Table S2L. Spin Contamination Values From BSS Calculation and Yamaguchi Correction[1,2] BSS Energy of **2**. Using $<S^2>$ values and energies for the triplet and BSS solutions for the same geometry, $\alpha = <S^2>_{trip.}/(<S^2>_{trip.} - <S^2>_{BSS})$, $\beta = <S^2>_{BSS}/(<S^2>_{trip.} - <S^2>_{BSS})$, and $E_{Yamaguchi} = \alpha E_{BSS} - \beta E_{trip}$.

Ni–C Dist. (Å)	$<S^2>$ S=1	$<S^2>$ BSS	α	β	Energy S=1/ kcal mol^{-1}	Energy BSS/ kcal mol^{-1}	Energy Yamaguchi/ kcal mol^{-1}
1.89	2.01	0.00	1.00	0.00	37.5	0.0	0.0
2.02	2.01	0.00	1.00	0.00	34.6	1.5	1.5
2.21	2.01	0.00	1.00	0.00	36.7	8.8	8.8
2.40	2.01	0.00	1.00	0.00	41.7	18.3	18.3
2.60	2.01	0.03	1.02	0.02	47.0	27.6	27.2
2.91	2.04	0.50	1.33	0.33	51.7	39.6	35.6
3.14	2.04	0.94	1.86	0.86	42.9	44.5	45.9
3.31	2.04	0.98	1.93	0.93	44.3	45.4	46.4
3.49	2.03	1.00	1.98	0.98	44.8	45.5	46.2
3.71	2.03	1.02	2.00	1.00	44.8	45.3	45.7
3.94	2.03	1.02	2.02	1.02	44.6	44.9	45.1

E. Figures Part 2: Compound *2*

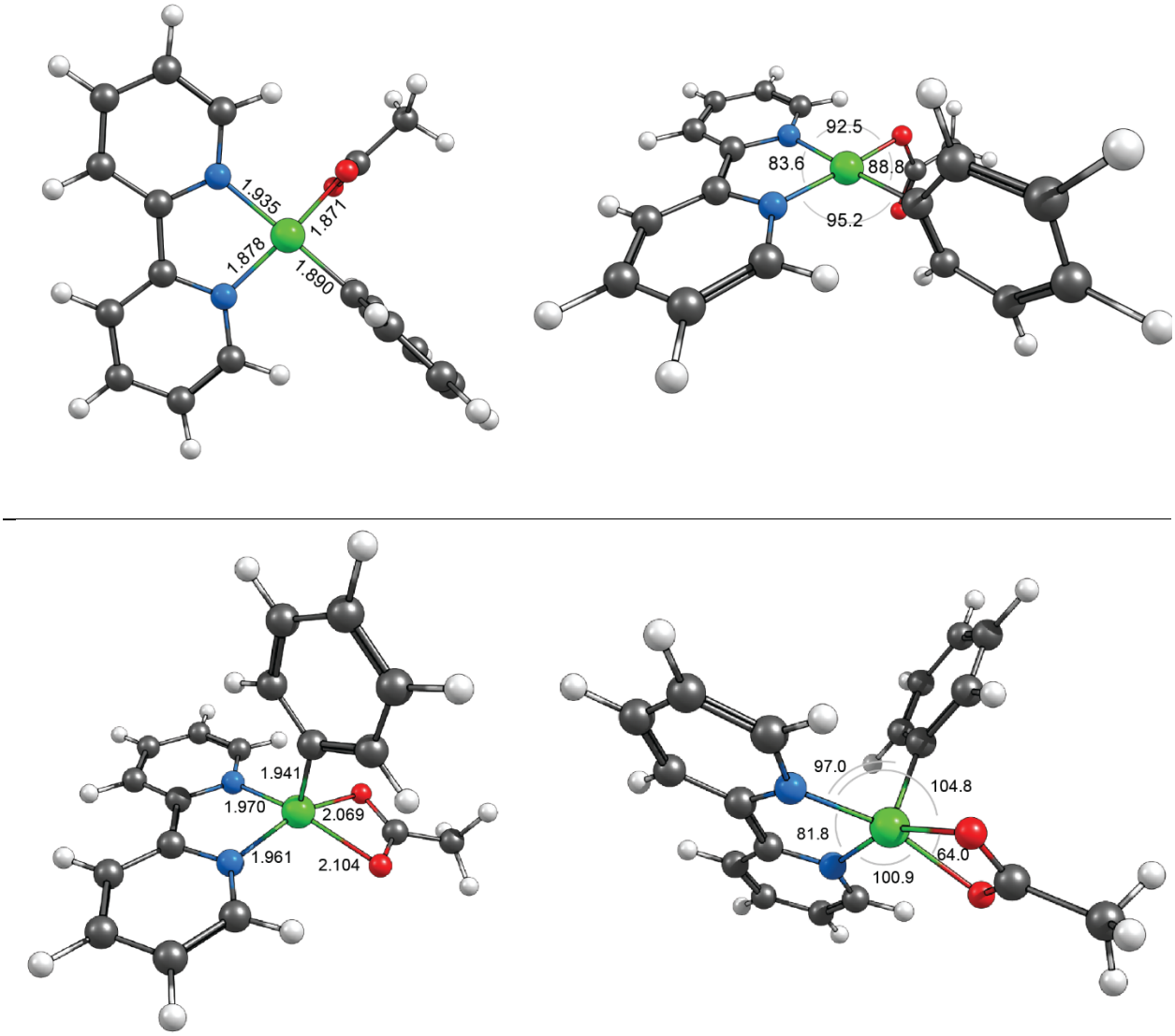


Figure S2A. Top: square planar equilibrium geometry of compound **2** (S=0), and bottom: square pyramidal equilibrium geometry of **2** (S=1) as calculated by DFT. Selected bond lengths and angles are shown.

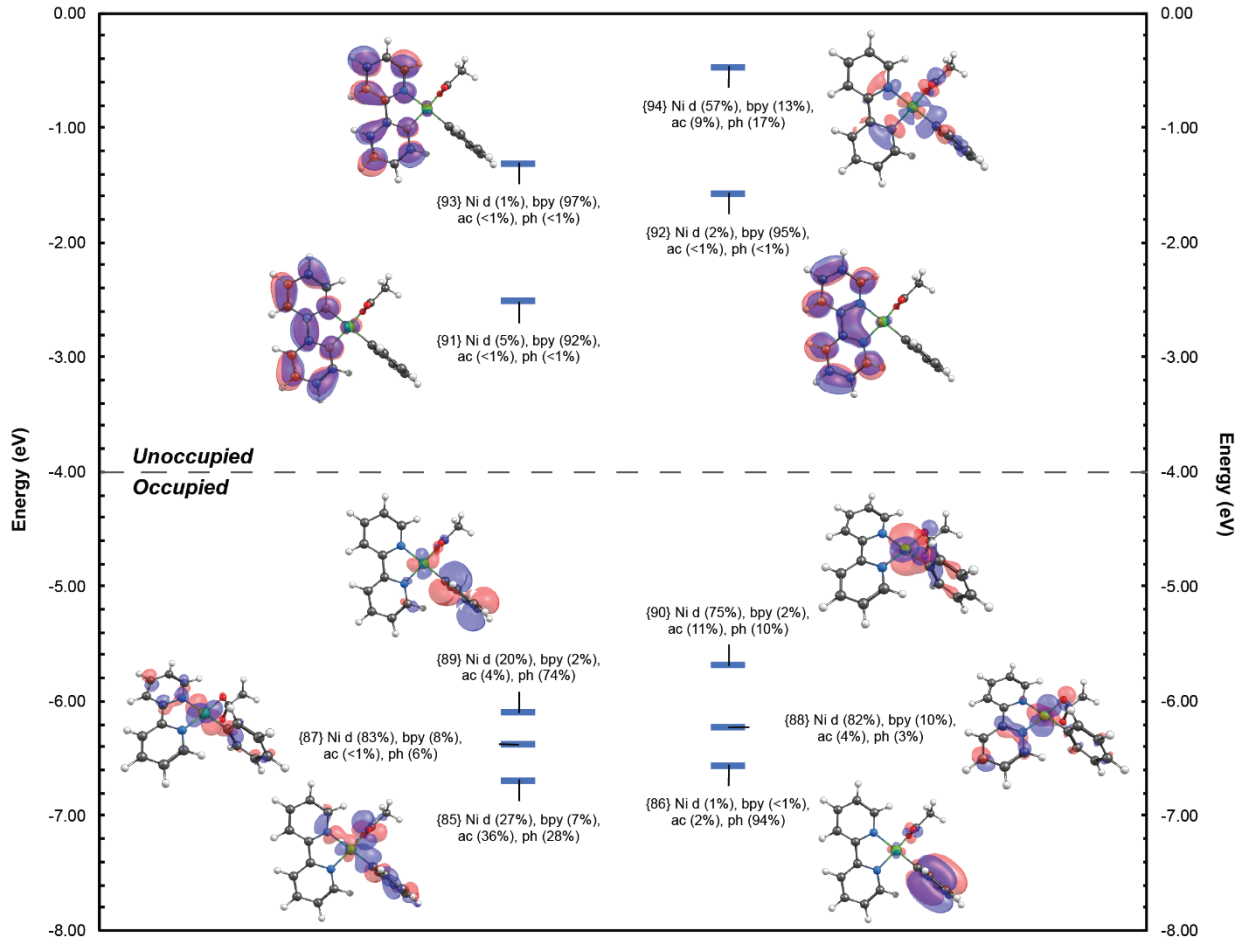


Figure S2B. Compound **2** (S=0)– Single point DFT Frontier molecular orbital diagram. Orbitals are offset for clarity.

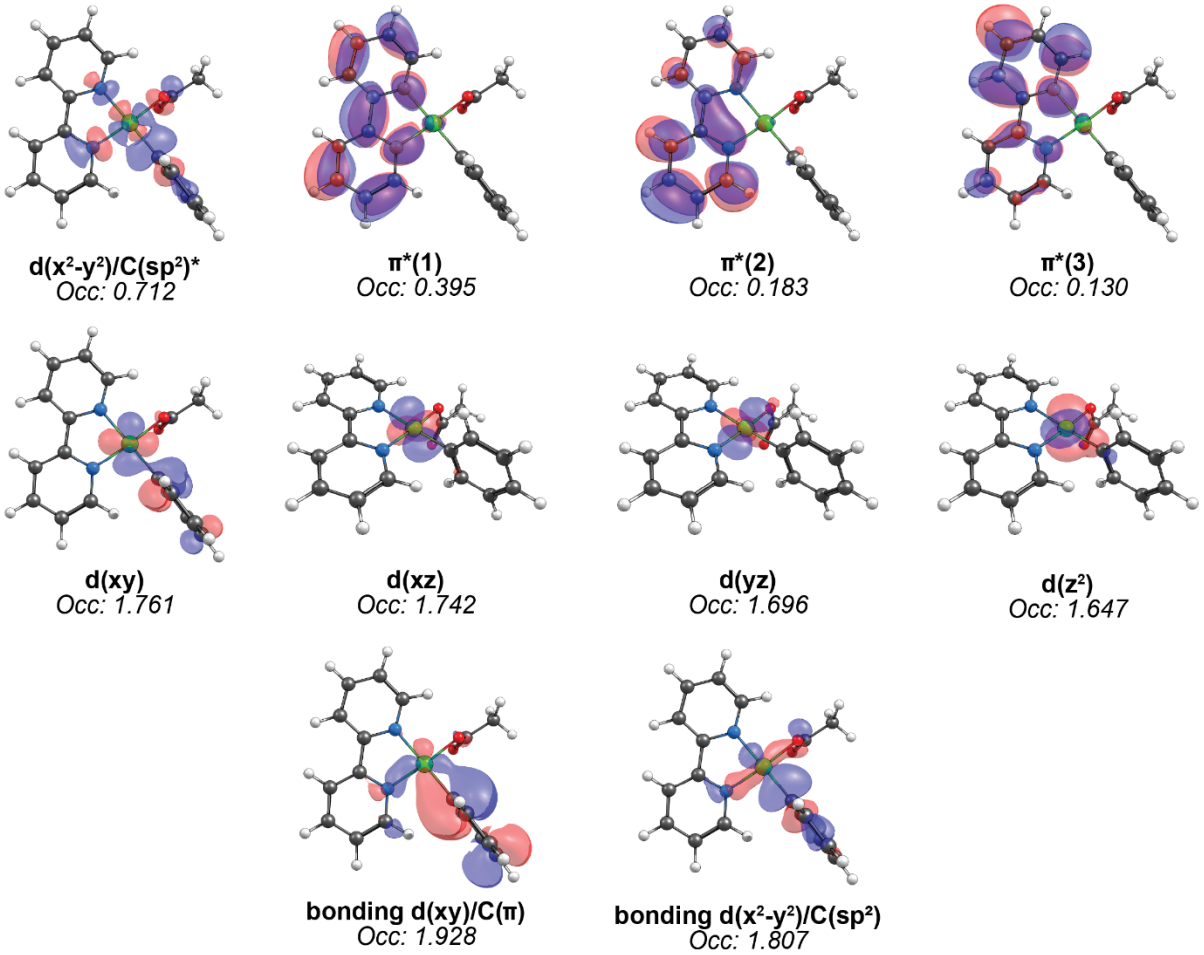


Figure S2C. Compound **2** (S=0)– CASSCF/QD-NEVPT2 10o, 12e Active Space.

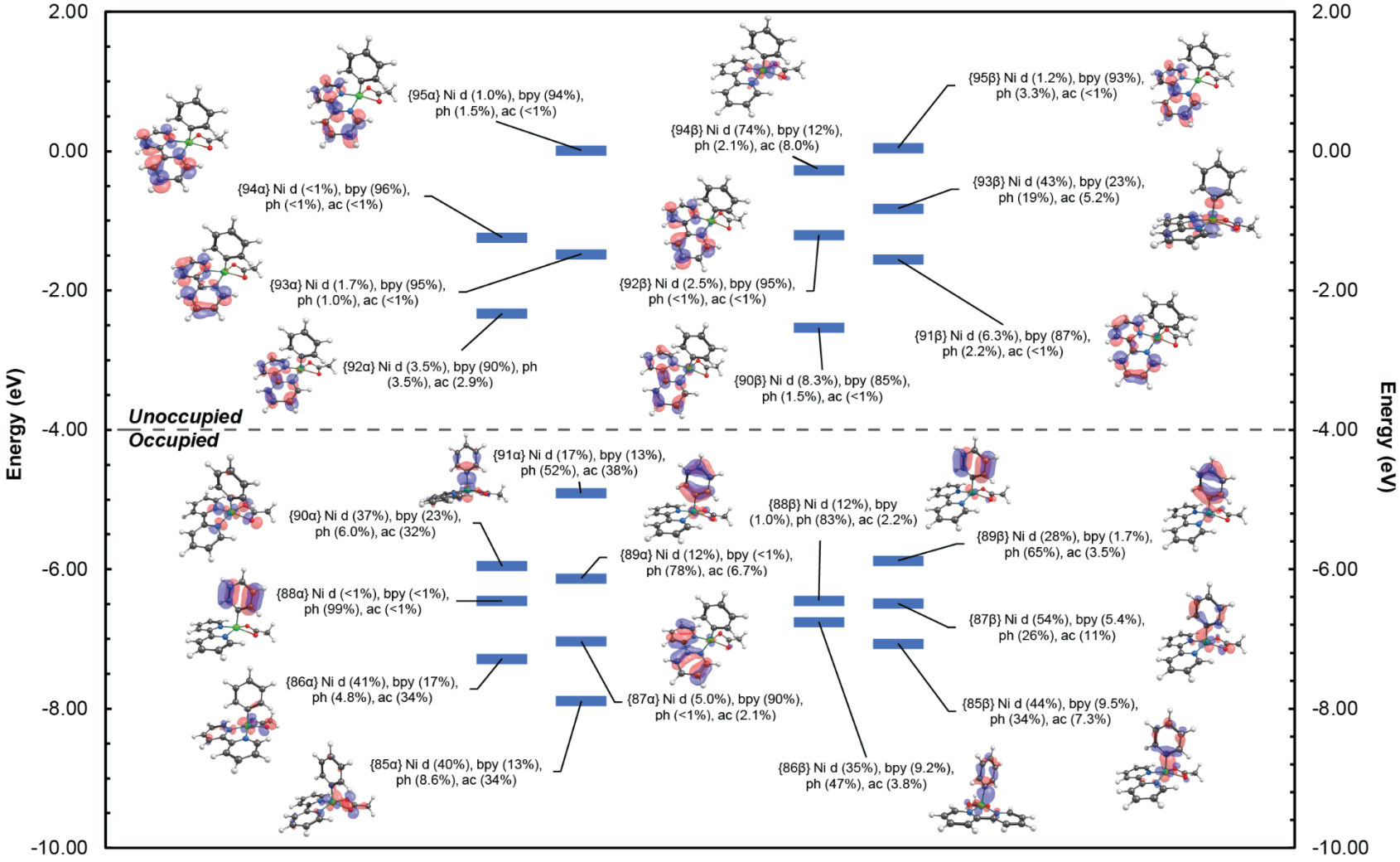


Figure S2D. Compound **2** (S=1) – Single point DFT Frontier molecular orbital diagram, with α orbitals on the left and β orbitals on the right. α and β orbitals are also offset for clarity.

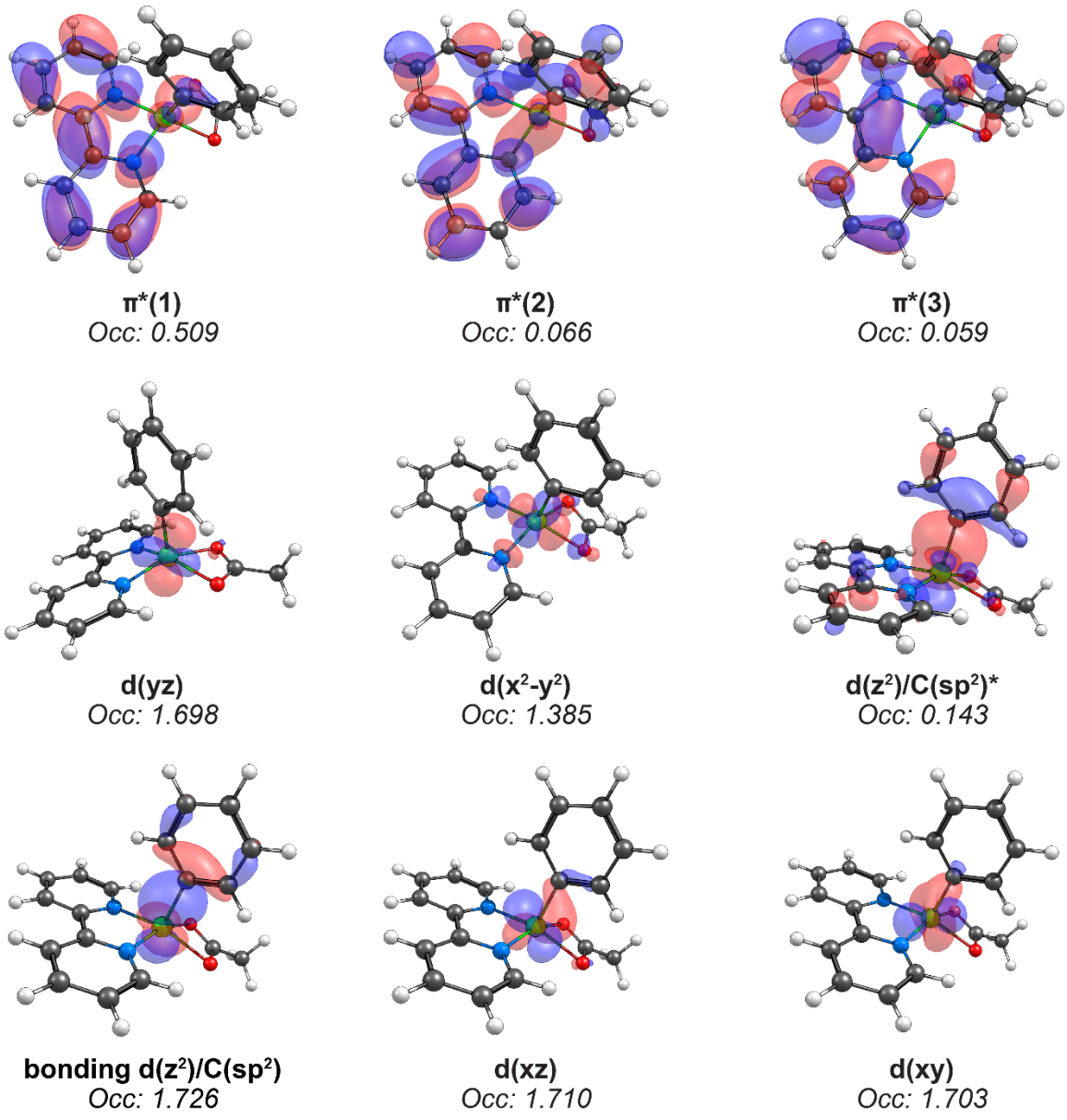


Figure S2E. Compound **2** (S=1) – CASSCF/QD-NEVPT2 9o, 10e Active Space.

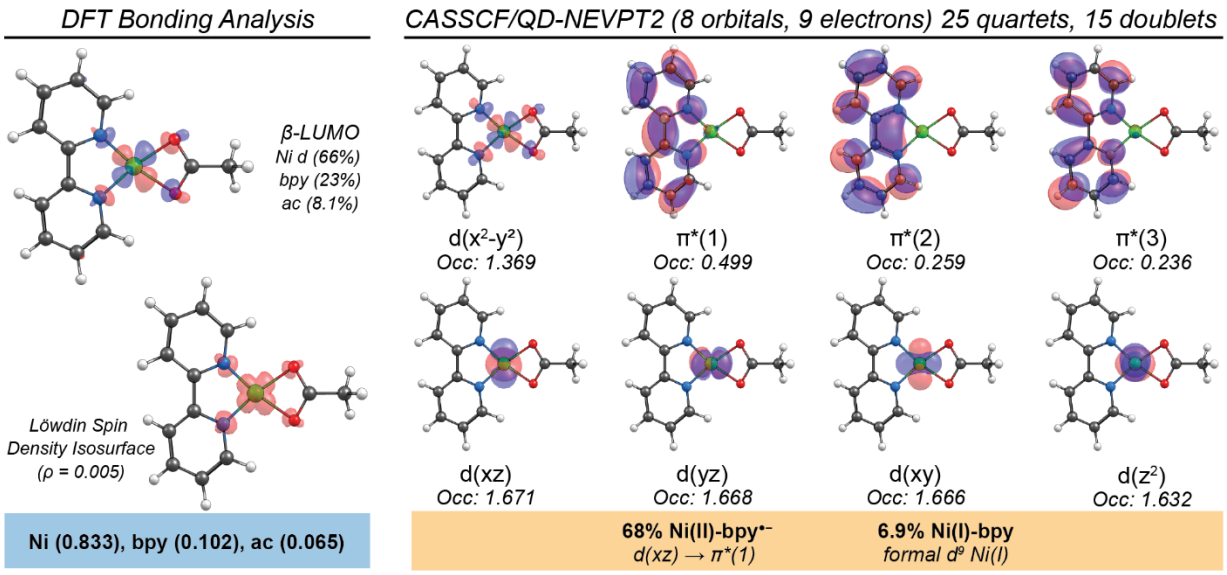


Figure S2F. Comparison between the description given by DFT vs CASSCF/QD-NEVPT2 of the formal Ni(I) product of **2** that results after Ni–C bond cleavage.

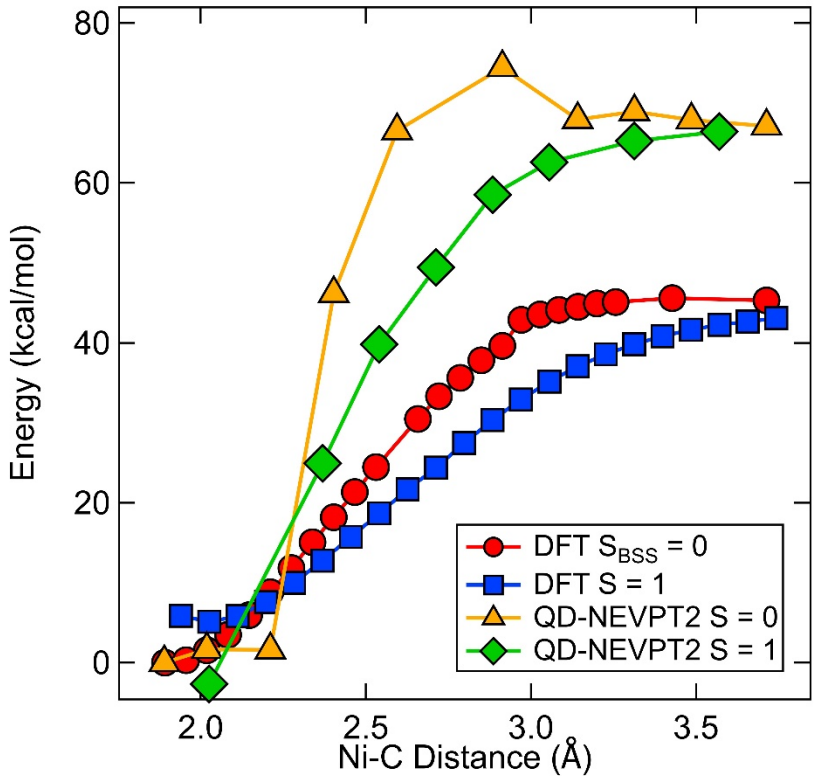


Figure S2G. Thermodynamics (DFT and CASSCF/QDNEVPT2) along Ni–C coordinate for **2**.

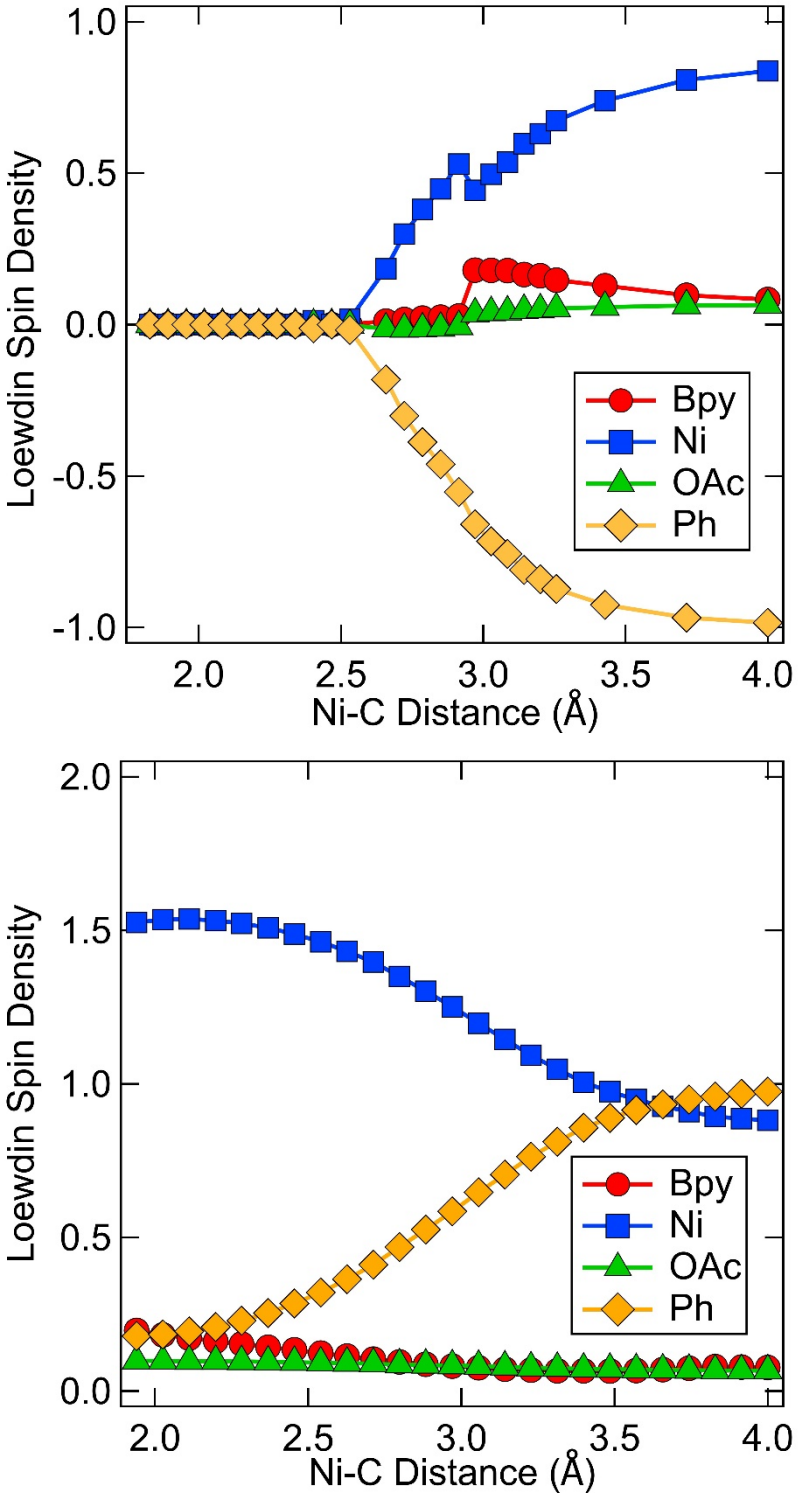


Figure S2H. DFT Loewdin spin density per group along the Ni–C coordinate for **2**: (top) BSS and (bottom) UKS S=1.

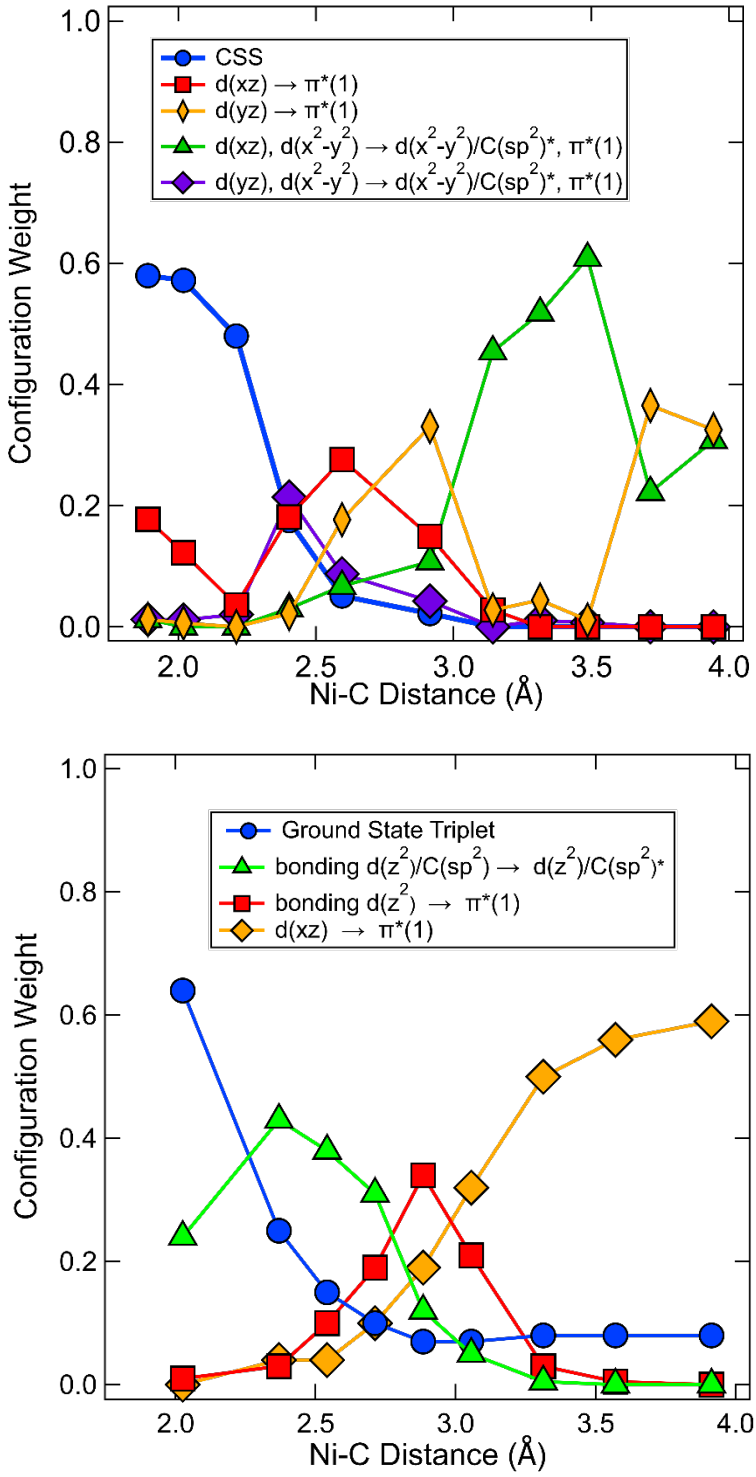


Figure S2I. Dominant CASSCF/QD-NEVPT2 CI vectors along the Ni–C coordinate for **2**: (top) S=0 and (bottom) S=1. Note that for high spin **2**, the ground state triplet is $[d(x^2\text{-}y^2)]^1[(dz^2)/C(sp^2)^*]^1$, making a d(xz) → π*(1) transition yield a configuration of $[d(xz)]^1[d(x^2\text{-}y^2)]^1[(dz^2)/C(sp^2)^*]^1[\pi^*(1)]^1$.

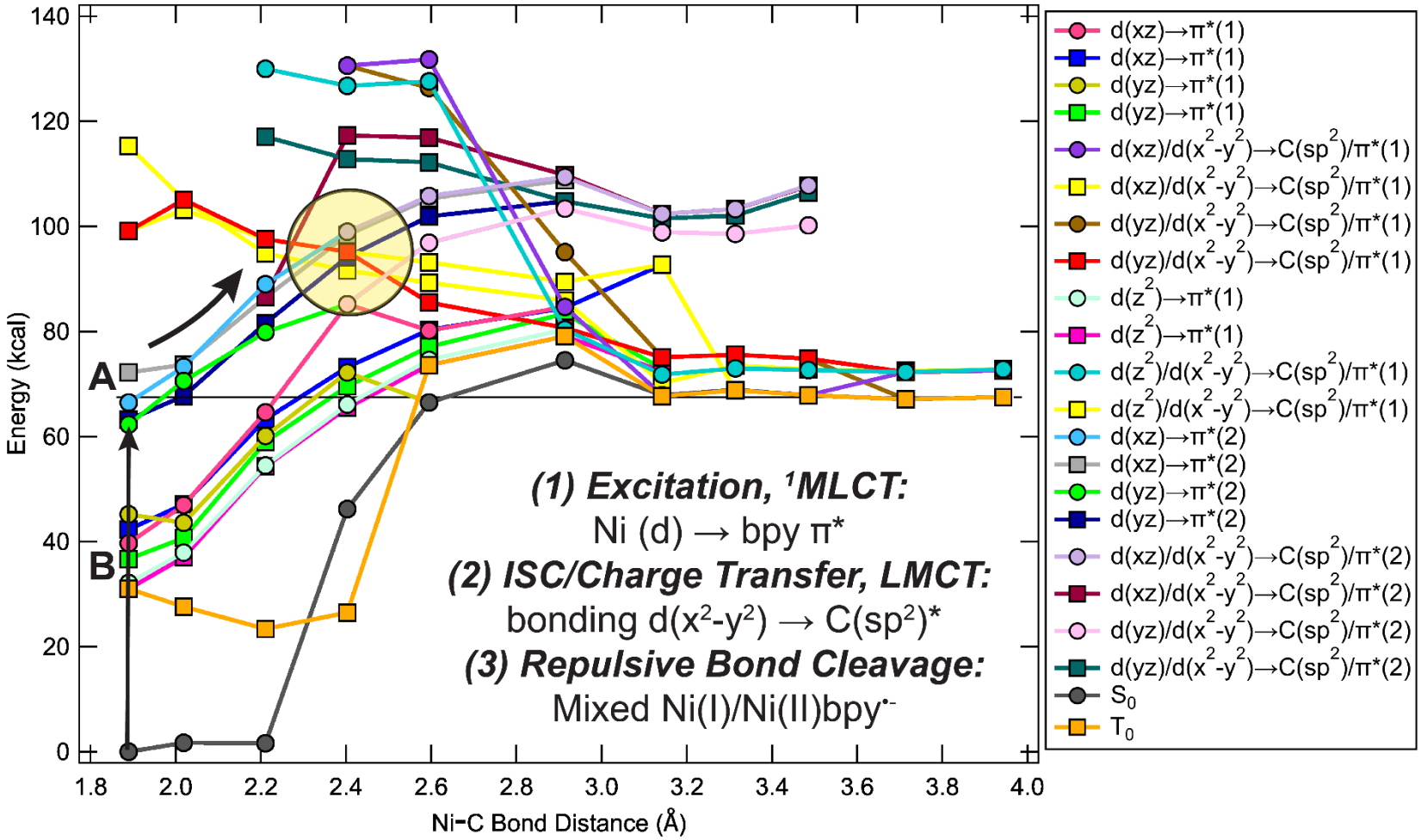


Figure S2J. CASSCF/QD-NEVPT2 calculated relaxed ground and excited state PESs along the Ni–C coordinate of **2**, with depictions of vertical excitation (black vertical arrow), the higher (A) and lower energy (B) manifolds of MLCTs, and the crossings between the higher energy MLCTs and the repulsive triplet surfaces (circled). Singlet states are shown with circles, triplets with squares.

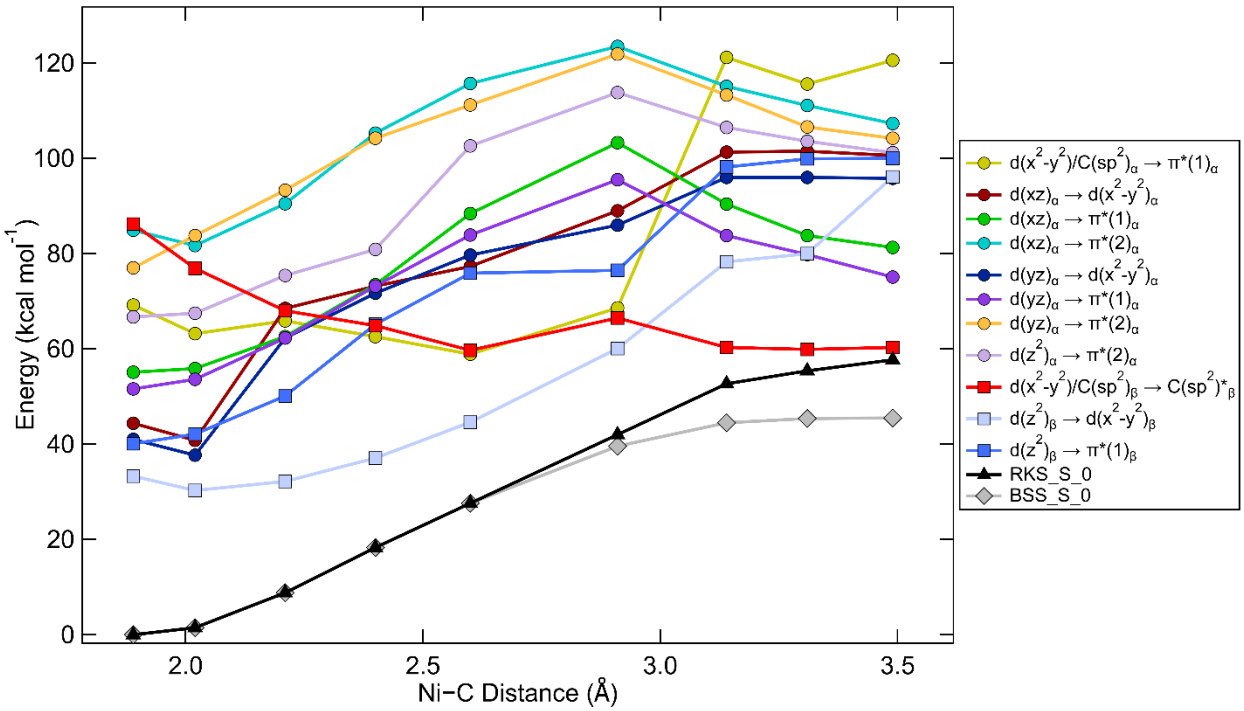


Figure S2K. Broken symmetry singlet TDDFT (CPCM(THF)) excitations along the Ni–C coordinate of **2** show a possible high energy reuplusive state (red line) which is ~86 kcal mol^{-1} above the equilibrium ground state. Spin-contaminated BSS calculations gave a Ni–C BDE of 45.1 kcal mol^{-1}, while the Yamaguchi corrected Ni–C BDE is essentially identical, at 44.9 kcal mol^{-1}.

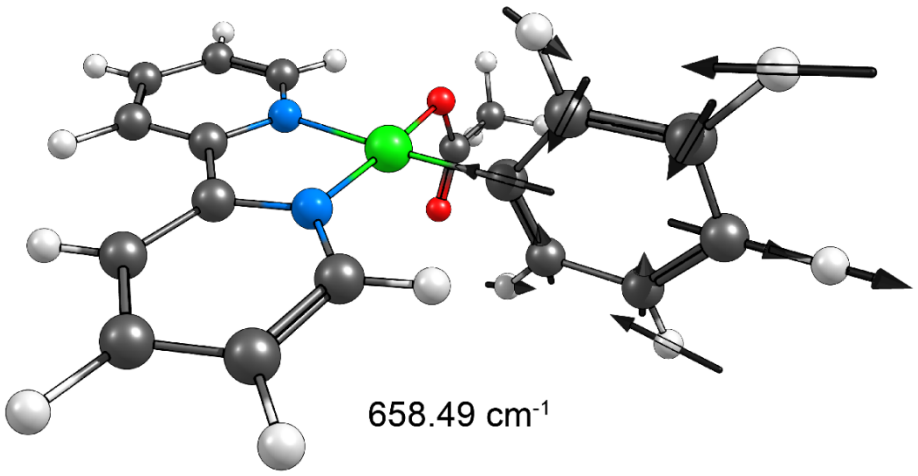


Figure S2L. Higher energy vibrational frequency in **2** that exhibits a Ni–C bond stretching mode.

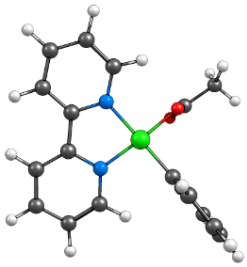
References

(1) Yamaguchi, K.; Takahara, Y.; Fueno, T.; Houk, K. N. Extended Hartree-Fock (EHF) Theory of Chemical Reactions. *Theor. Chim. Acta* **1988**, *73* (5), 337–364. https://doi.org/10.1007/BF00527740.

(2) Kitagawa, Y.; Saito, T.; Nakanishi, Y.; Kataoka, Y.; Matsui, T.; Kawakami, T.; Okumura, M.; Yamaguchi, K. Spin Contamination Error in Optimized Geometry of Singlet Carbene ($^1A_1$) by Broken-Symmetry Method. *J. Phys. Chem. A* **2009**, *113* (52), 15041–15046. https://doi.org/10.1021/jp905125g.

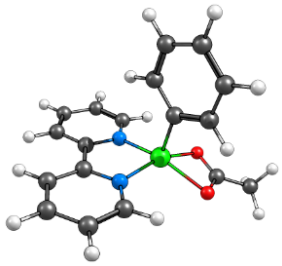
(3) Shields, B. J.; Kudisch, B.; Scholes, G. D.; Doyle, A. G. Long-Lived Charge-Transfer States of Nickel(II) Aryl Halide Complexes Facilitate Bimolecular Photoinduced Electron Transfer. *J. Am. Chem. Soc.* **2018**, *140* (8), 3035–3039. https://doi.org/10.1021/jacs.7b13281.

Appendix: DFT Optimized Structures



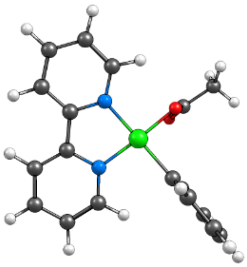
39
Aryl Carboxylate RKS Fully Optimized

6	-4.707452000	-0.391161000	0.168879000
6	-3.865012000	-1.497580000	0.038873000
6	-4.140109000	0.887035000	0.255790000
6	-2.752713000	1.016088000	0.200045000
7	-1.933587000	-0.047766000	0.060734000
6	-2.478609000	-1.298990000	-0.008334000
6	-1.460971000	-2.349273000	-0.118250000
7	-0.166326000	-1.869074000	-0.070411000
6	-1.739446000	-3.714239000	-0.251538000
1	-4.283526000	-2.504491000	-0.019809000
1	-5.791392000	-0.525529000	0.206513000
1	-4.762552000	1.777733000	0.365224000
1	-2.236770000	1.976265000	0.267990000
6	-0.692669000	-4.632557000	-0.340510000
1	-2.776288000	-4.054539000	-0.291989000
6	0.619531000	-4.146965000	-0.292636000
1	-0.896634000	-5.700614000	-0.447096000
6	0.841181000	-2.778203000	-0.162330000
1	1.478057000	-4.818827000	-0.358493000
1	1.846792000	-2.360476000	-0.125912000
28	0.000000000	0.000000000	0.000000000
6	1.888574000	0.000000000	0.071467000
8	0.037451000	1.868881000	0.070582000
6	0.190929000	2.451672000	-1.106243000
8	0.225110000	1.869891000	-2.193488000
6	0.355279000	3.966397000	-1.002699000
1	-0.049934000	4.368839000	-0.064071000
1	-0.117221000	4.453549000	-1.867090000
1	1.431644000	4.201813000	-1.034290000
6	2.681131000	0.110776000	-1.086655000
6	2.532134000	-0.141112000	1.316068000
6	3.933034000	-0.191744000	1.400485000
6	4.712671000	-0.100446000	0.240291000
6	4.082032000	0.055110000	-1.001171000
1	2.200016000	0.268814000	-2.055522000
1	4.682463000	0.143756000	-1.913297000
1	5.804646000	-0.139214000	0.304678000
1	1.944695000	-0.207871000	2.238925000
1	4.414754000	-0.298307000	2.378800000



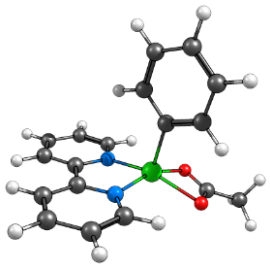
39
Aryl Carboxylate Triplet Fully Optimized

C	-4.628182267	0.538495192	-0.961576888
C	-4.036390125	-0.716285517	-0.828856077
C	-3.827429540	1.689473586	-0.844136718
C	-2.466522118	1.536018327	-0.598002976
N	-1.885355862	0.321777139	-0.473131211
C	-2.655468845	-0.808316711	-0.582965994
C	-1.899132774	-2.055341059	-0.419720306
N	-0.551359209	-1.866233900	-0.239020821
C	-2.451445311	-3.347481997	-0.428190764
H	-4.642029460	-1.621030291	-0.918182042
H	-5.700453833	0.624361759	-1.154767210
H	-4.254050305	2.690045265	-0.943217439
H	-1.786231644	2.385811418	-0.497655678
C	-1.618281973	-4.452618667	-0.267591134
H	-3.527480140	-3.485483993	-0.556753202
C	-0.238083683	-4.246424965	-0.090286737
H	-2.034211972	-5.463163278	-0.274413057
C	0.249010194	-2.943969868	-0.074692325
H	0.449428677	-5.085749941	0.035303239
H	1.308656802	-2.717886913	0.066591713
Ni	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	1.941270076
O	0.836868028	1.835220159	-0.459862035
C	1.977186221	1.263314296	-0.559828537
O	2.069773772	0.000000000	-0.379413077
C	3.209901395	2.084526129	-0.855420462
H	2.957051335	2.951952712	-1.480186754
H	3.980962289	1.472020444	-1.341478363
H	3.622881992	2.464069701	0.093678092
C	1.204997611	-0.265392124	2.617918715
C	-1.153541560	0.231472608	2.709904277
C	-1.104433709	0.219800043	4.113437424
C	0.102407966	-0.036987929	4.774486362
C	1.257347547	-0.280109218	4.021031951
H	2.120750551	-0.448127948	2.047164672
H	2.209233659	-0.482775928	4.524868671
H	0.142543927	-0.048147070	5.868267772
H	-2.114785794	0.434005254	2.225455631
H	-2.016591837	0.412088491	4.689700490



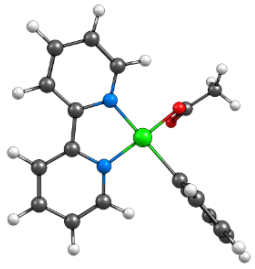
39
Aryl Carboxylate RKS 2.0 Å Ni–C distance

6	-4.693690000	-0.377607000	0.208141000
6	-3.854927000	-1.487845000	0.085423000
6	-4.122191000	0.900456000	0.268838000
6	-2.735425000	1.026280000	0.197011000
7	-1.919905000	-0.042136000	0.065034000
6	-2.469004000	-1.294077000	0.018640000
6	-1.454282000	-2.346522000	-0.092158000
7	-0.159670000	-1.864447000	-0.063635000
6	-1.732600000	-3.712503000	-0.211972000
1	-4.275847000	-2.494799000	0.047034000
1	-5.777362000	-0.508728000	0.260458000
1	-4.741255000	1.794336000	0.371448000
1	-2.216058000	1.985699000	0.246974000
6	-0.685062000	-4.629431000	-0.309868000
1	-2.769328000	-4.054693000	-0.236214000
6	0.626916000	-4.141422000	-0.285373000
1	-0.888556000	-5.698538000	-0.406233000
6	0.848774000	-2.771420000	-0.165918000
1	1.485399000	-4.812332000	-0.360653000
1	1.853427000	-2.350398000	-0.145195000
28	0.000000000	0.000000000	0.000000000
6	2.017685000	0.000000000	0.084979000
8	0.052094000	1.865249000	0.070135000
6	0.261577000	2.450291000	-1.097058000
8	0.329276000	1.872299000	-2.184483000
6	0.449054000	3.961064000	-0.977444000
1	-0.018794000	4.370609000	-0.071441000
1	0.054955000	4.459146000	-1.874048000
1	1.529372000	4.173332000	-0.922681000
6	2.806700000	0.141022000	-1.068122000
6	2.648874000	-0.161636000	1.329587000
6	4.050421000	-0.200158000	1.420206000
6	4.833231000	-0.076418000	0.265035000
6	4.208332000	0.097402000	-0.977005000
1	2.325914000	0.312631000	-2.034689000
1	4.812917000	0.209702000	-1.883759000
1	5.925280000	-0.105543000	0.333930000
1	2.055300000	-0.253714000	2.246171000
1	4.529567000	-0.322386000	2.397970000



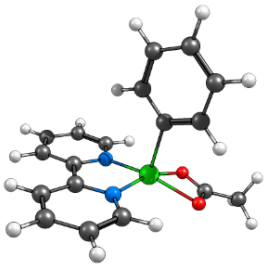
39
Aryl Carboxylate Triplet 2.0 Å Ni–C distance

C	4.652962138	0.247672215	-0.960748872
C	3.858692324	1.385132560	-0.827625658
C	4.057100421	-1.021601326	-0.843960973
C	2.689729649	-1.099243568	-0.598133452
N	1.912595075	0.000000000	-0.473178628
C	2.481802482	1.243488749	-0.582375541
C	1.526490367	2.345598338	-0.419358073
N	0.229634267	1.932361247	-0.239382774
C	1.853706499	3.712207257	-0.427210765
H	4.303699342	2.378801972	-0.916477083
H	5.724444066	0.343521623	-1.153633587
H	4.645958714	-1.936104285	-0.943246646
H	2.161989463	-2.051349421	-0.498170852
C	0.846356613	4.661432164	-0.267123269
H	2.891320837	4.029240368	-0.554737258
C	-0.479645928	4.226007569	-0.091062692
H	1.086525305	5.727512033	-0.273378287
C	-0.740747906	2.860136941	-0.075816723
H	-1.298583365	4.937797875	0.033908133
H	-1.747396249	2.459066739	0.064654992
Ni	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	2.025833398
O	-0.516235484	-1.949939411	-0.459210797
C	-1.736503645	-1.578212110	-0.559195131
O	-2.040268981	-0.348344554	-0.379327501
C	-2.813835266	-2.594882492	-0.854191895
H	-2.419601513	-3.407396504	-1.479472468
H	-3.677155262	-2.120378922	-1.339275366
H	-3.156237996	-3.038468724	0.095266302
C	-1.232470985	0.061798980	2.702298513
C	1.175882678	-0.036629647	2.794683615
C	1.125319354	-0.033305245	4.198219072
C	-0.107531611	0.019487328	4.859078134
C	-1.286691340	0.067585931	4.105440848
H	-2.165779319	0.090001930	2.131454940
H	-2.259113953	0.109418148	4.609077483
H	-0.149116328	0.023721355	5.952855194
H	2.157434700	-0.076313461	2.310253531
H	2.056707289	-0.071442599	4.774543371



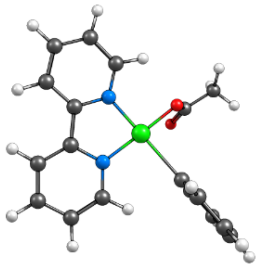
39
Aryl Carboxylate RKS 2.2 Å Ni–C distance

6	-4.667690000	-0.340216000	0.399001000
6	-3.834751000	-1.460232000	0.340554000
6	-4.093105000	0.936002000	0.325213000
6	-2.710527000	1.050861000	0.188883000
7	-1.900876000	-0.029012000	0.118851000
6	-2.452735000	-1.279613000	0.203189000
6	-1.443466000	-2.340459000	0.136965000
7	-0.150389000	-1.857802000	0.075468000
6	-1.721836000	-3.711431000	0.131440000
1	-4.256663000	-2.465399000	0.406745000
1	-5.748464000	-0.461773000	0.505220000
1	-4.707209000	1.837899000	0.373320000
1	-2.188234000	2.008557000	0.135640000
6	-0.675153000	-4.631715000	0.054800000
1	-2.757221000	-4.055577000	0.177954000
6	0.634777000	-4.142788000	-0.017480000
1	-0.878170000	-5.705228000	0.047430000
6	0.857419000	-2.767490000	-0.007486000
1	1.491064000	-4.817459000	-0.083340000
1	1.859289000	-2.342582000	-0.060260000
28	0.000000000	0.000000000	0.000000000
6	2.210107000	0.000000000	0.068146000
8	0.074219000	1.860972000	-0.064346000
6	0.332518000	2.353160000	-1.264029000
8	0.422543000	1.692127000	-2.301484000
6	0.550808000	3.864041000	-1.250899000
1	0.037046000	4.353341000	-0.411606000
1	0.226165000	4.297101000	-2.206939000
1	1.630313000	4.058354000	-1.141099000
6	2.971220000	0.113324000	-1.102453000
6	2.850501000	-0.117764000	1.308629000
6	4.254430000	-0.140120000	1.379426000
6	5.017579000	-0.042891000	0.208673000
6	4.375204000	0.086342000	-1.029904000
1	2.471408000	0.249395000	-2.064842000
1	4.967101000	0.176188000	-1.947554000
1	6.110802000	-0.058803000	0.262541000
1	2.268332000	-0.188293000	2.234054000
1	4.750248000	-0.228379000	2.352605000



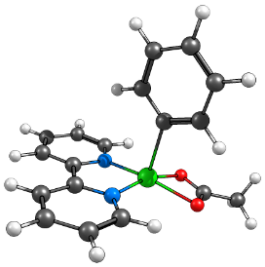
39
Aryl Carboxylate Triplet 2.2 Å Ni–C distance

C	4.692842251	0.243448950	-0.673192936
C	3.893960871	1.382385145	-0.574593034
C	4.088687563	-1.023608091	-0.602009839
C	2.708182227	-1.099817676	-0.438355225
N	1.927429704	0.000000000	-0.348712378
C	2.506212156	1.241182483	-0.409963344
C	1.545042921	2.346652362	-0.281769430
N	0.243903154	1.932936002	-0.152741106
C	1.875141420	3.711355013	-0.268997848
H	4.345938815	2.375557190	-0.624960397
H	5.773901983	0.338615433	-0.802325139
H	4.680267902	-1.938973987	-0.673731656
H	2.173993051	-2.051576885	-0.377266195
C	0.863328261	4.661494134	-0.135677401
H	2.916723004	4.027975884	-0.359574183
C	-0.466899457	4.226694283	-0.009003596
H	1.105200201	5.727152781	-0.125261999
C	-0.730523809	2.860236717	-0.017602335
H	-1.288570248	4.938579947	0.096296870
H	-1.741833015	2.458825699	0.083293418
Ni	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	2.197500429
O	-0.536904347	-1.943675784	-0.430091582
C	-1.758921921	-1.566314538	-0.455967846
O	-2.041940901	-0.331157593	-0.272071153
C	-2.859809208	-2.578310207	-0.666047091
H	-2.522979478	-3.384568968	-1.331940944
H	-3.761474175	-2.098401716	-1.068734024
H	-3.116671995	-3.032993284	0.304858135
C	-1.238215885	0.057306671	2.849842482
C	1.174446651	-0.031449408	2.957346771
C	1.115457604	-0.018213462	4.361872019
C	-0.123663664	0.034419658	5.012111005
C	-1.300896379	0.071949651	4.253877591
H	-2.164770989	0.079591638	2.267185310
H	-2.274962260	0.112345414	4.754810681
H	-0.171681095	0.045570898	6.105699091
H	2.156121867	-0.073288968	2.472046127
H	2.041782018	-0.049648609	4.947045036



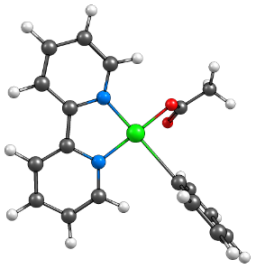
39
Aryl Carboxylate RKS 2.4 Å Ni–C distance

6	-4.669212000	-0.337664000	0.196995000
6	-3.832856000	-1.456448000	0.227003000
6	-4.093614000	0.935805000	0.087977000
6	-2.706864000	1.049996000	0.006576000
7	-1.893561000	-0.030042000	0.023002000
6	-2.446630000	-1.278690000	0.141548000
6	-1.433325000	-2.337617000	0.162176000
7	-0.141112000	-1.850691000	0.135718000
6	-1.704594000	-3.709439000	0.196183000
1	-4.255532000	-2.459105000	0.321502000
1	-5.753365000	-0.457696000	0.261950000
1	-4.710693000	1.836751000	0.066825000
1	-2.183616000	2.005795000	-0.068698000
6	-0.650147000	-4.624377000	0.194686000
1	-2.739135000	-4.058950000	0.213248000
6	0.659410000	-4.130649000	0.154167000
1	-0.847107000	-5.698782000	0.219029000
6	0.875484000	-2.754353000	0.123031000
1	1.520483000	-4.802344000	0.145354000
1	1.875031000	-2.321633000	0.094835000
28	0.000000000	0.000000000	0.000000000
6	2.391834000	0.000000000	0.229742000
8	0.092403000	1.854557000	-0.125019000
6	0.483230000	2.288894000	-1.310912000
8	0.665197000	1.577545000	-2.302402000
6	0.723712000	3.795429000	-1.343664000
1	0.116586000	4.331241000	-0.600578000
1	0.528445000	4.183464000	-2.352641000
1	1.783759000	3.983661000	-1.106960000
6	3.205034000	0.103799000	-0.902325000
6	2.956788000	-0.097039000	1.504587000
6	4.356100000	-0.105794000	1.650303000
6	5.178791000	-0.015907000	0.520046000
6	4.604057000	0.090098000	-0.753643000
1	2.753735000	0.217064000	-1.890967000
1	5.244262000	0.170701000	-1.639257000
1	6.267670000	-0.021476000	0.632613000
1	2.324283000	-0.161514000	2.396650000
1	4.800214000	-0.177361000	2.649599000



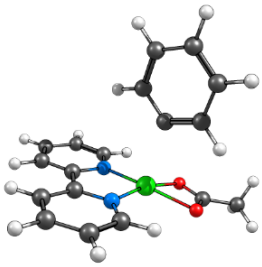
39
Aryl Carboxylate Triplet 2.4 Å Ni–C distance

C	4.705912086	0.243429899	-0.532806844
C	3.904978049	1.382433130	-0.443768400
C	4.099339420	-1.022842819	-0.489291360
C	2.714416756	-1.099405743	-0.363531767
N	1.932270860	0.000000000	-0.282900696
C	2.514161271	1.240425754	-0.315961048
C	1.550360583	2.346604217	-0.196454391
N	0.248057265	1.931468823	-0.092422757
C	1.880954620	3.710196364	-0.166436126
H	4.358728981	2.375669463	-0.471718960
H	5.790053046	0.338926339	-0.632385365
H	4.691922813	-1.938165213	-0.553225397
H	2.178527664	-2.051396355	-0.325731645
C	0.867026105	4.659738637	-0.038592697
H	2.923737043	4.027383520	-0.239350423
C	-0.464208569	4.224095195	0.064057138
H	1.108937233	5.725152221	-0.014117777
C	-0.728217100	2.857462688	0.036243295
H	-1.287163353	4.935042448	0.165853949
H	-1.740878634	2.454988225	0.117565906
Ni	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	2.369167217
O	-0.548099175	-1.939838356	-0.410363773
C	-1.769502225	-1.559543571	-0.395139553
O	-2.041812984	-0.322185199	-0.208296562
C	-2.879745113	-2.569431078	-0.559774334
H	-2.570848400	-3.377414376	-1.237078053
H	-3.795720107	-2.088569473	-0.927445310
H	-3.098639536	-3.022265390	0.421197000
C	-1.243583104	0.052514568	3.004505843
C	1.172430745	-0.028760456	3.126433206
C	1.104443106	-0.013021677	4.531426115
C	-0.139834900	0.036816220	5.172691256
C	-1.314056744	0.069185674	4.408990596
H	-2.165268990	0.071853329	2.413668786
H	-2.290563897	0.106886388	4.905575603
H	-0.194313321	0.049388008	6.265984983
H	2.155411989	-0.068976919	2.643072968
H	2.026649227	-0.040759697	5.123450598



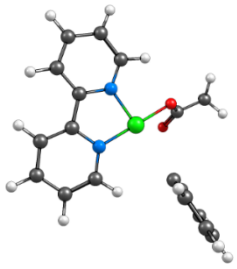
39
Aryl Carboxylate RKS 2.6 Å Ni–C distance

6	-4.650982000	-0.407914000	0.330148000
6	-3.801992000	-1.515781000	0.265619000
6	-4.093534000	0.877183000	0.273942000
6	-2.712136000	1.014349000	0.149994000
7	-1.887326000	-0.054819000	0.074642000
6	-2.421979000	-1.316088000	0.140046000
6	-1.396756000	-2.361123000	0.061803000
7	-0.112354000	-1.855567000	0.025374000
6	-1.648968000	-3.736239000	0.017867000
1	-4.209724000	-2.527661000	0.318729000
1	-5.730593000	-0.545373000	0.427597000
1	-4.720863000	1.769731000	0.326659000
1	-2.202225000	1.979540000	0.111809000
6	-0.582685000	-4.632779000	-0.076133000
1	-2.677631000	-4.102054000	0.046260000
6	0.718589000	-4.118236000	-0.128833000
1	-0.764593000	-5.709476000	-0.112974000
6	0.916090000	-2.739606000	-0.078981000
1	1.587192000	-4.775344000	-0.208724000
1	1.907678000	-2.288387000	-0.110176000
28	0.000000000	0.000000000	0.000000000
6	2.586202000	0.000000000	0.207671000
8	0.078132000	1.858565000	-0.014305000
6	0.487561000	2.352695000	-1.169975000
8	0.697856000	1.687613000	-2.187961000
6	0.722238000	3.859301000	-1.125697000
1	0.083792000	4.358747000	-0.383432000
1	0.563921000	4.291909000	-2.122855000
1	1.771047000	4.040271000	-0.838729000
6	3.363817000	0.259947000	-0.922042000
6	3.179480000	-0.244047000	1.447356000
6	4.582611000	-0.245524000	1.557775000
6	5.374295000	0.000008000	0.428347000
6	4.766601000	0.253680000	-0.808757000
1	2.884231000	0.485808000	-1.877906000
1	5.383020000	0.455729000	-1.691979000
1	6.465617000	0.000474000	0.513975000
1	2.569650000	-0.429853000	2.338076000
1	5.053144000	-0.433244000	2.529639000



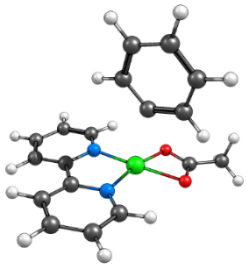
39
Aryl Carboxylate Triplet 2.7 Å Ni–C distance

C	4.693846108	0.253460832	-0.554366775
C	3.894627874	1.389045429	-0.406680804
C	4.089200320	-1.012810663	-0.530819618
C	2.707899416	-1.094912239	-0.366321697
N	1.928311319	0.000000000	-0.221828487
C	2.510556160	1.240647729	-0.235761798
C	1.548056697	2.342202156	-0.053801320
N	0.247098920	1.920279003	0.036678933
C	1.879225845	3.701559864	0.035714322
H	4.345658143	2.383799227	-0.425501266
H	5.774062049	0.353410905	-0.686665104
H	4.679710342	-1.925370431	-0.639115323
H	2.173835304	-2.048409509	-0.344781612
C	0.865655277	4.644460143	0.217130977
H	2.921709780	4.021606183	-0.029062563
C	-0.463319506	4.203240627	0.310064103
H	1.107569122	5.707593343	0.290509146
C	-0.728071917	2.838946343	0.217630101
H	-1.285603551	4.907746328	0.453960205
H	-1.739985656	2.432514233	0.286871132
Ni	0.000000000	0.000000000	0.000000000
C	0.000000000	0.000000000	2.712499828
O	-0.562161219	-1.930162793	-0.379252813
C	-1.781587404	-1.554084277	-0.278133807
O	-2.042874622	-0.317621379	-0.072952058
C	-2.896421410	-2.568344358	-0.364656728
H	-2.637305805	-3.368887967	-1.071146270
H	-3.840357075	-2.089350958	-0.655952928
H	-3.035958629	-3.031091487	0.626063913
C	-1.260563817	0.039697057	3.303476211
C	1.160266088	-0.025364584	3.480455571
C	1.058358005	-0.011459771	4.884649038
C	-0.202238258	0.028724381	5.495206525
C	-1.361178330	0.053740684	4.707385664
H	-2.166176973	0.053919817	2.687670735
H	-2.348001623	0.082647960	5.183926839
H	-0.281405115	0.038742472	6.586961699
H	2.151207571	-0.058982002	3.013027861
H	1.965965116	-0.033632154	5.499173690



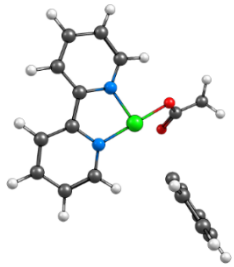
39
Aryl Carboxylate RKS 2.9 Å Ni–C distance

6	4.666210000	0.280284000	-0.003624000
6	3.845413000	1.410286000	-0.045116000
6	4.071357000	-0.990225000	-0.001114000
6	2.682488000	-1.091459000	-0.043028000
7	1.883612000	0.000000000	-0.096503000
6	2.455506000	1.248249000	-0.091074000
6	1.455926000	2.319683000	-0.144812000
7	0.160594000	1.850792000	-0.059783000
6	1.735042000	3.683916000	-0.280374000
1	4.282444000	2.411416000	-0.032863000
1	5.752888000	0.388692000	0.031889000
1	4.676983000	-1.898602000	0.034164000
1	2.145813000	-2.042948000	-0.030428000
6	0.683962000	4.600716000	-0.349135000
1	2.770914000	4.024010000	-0.346598000
6	-0.630492000	4.119151000	-0.289377000
1	0.886689000	5.669108000	-0.455166000
6	-0.854898000	2.751194000	-0.148834000
1	-1.486598000	4.794621000	-0.347873000
1	-1.854756000	2.321769000	-0.079978000
28	0.000000000	0.000000000	0.000000000
6	-2.791804000	0.202148000	0.810161000
8	-0.163798000	-1.861240000	0.060620000
6	-0.893088000	-2.264828000	-0.960505000
8	-1.315485000	-1.508715000	-1.845182000
6	-1.216127000	-3.752148000	-0.940863000
1	-0.404802000	-4.343560000	-0.493181000
1	-1.429859000	-4.104199000	-1.958792000
1	-2.118023000	-3.908451000	-0.326584000
6	-3.768013000	-0.126845000	-0.126357000
6	-3.116466000	0.607300000	2.101567000
6	-4.473462000	0.701657000	2.467215000
6	-5.472624000	0.386515000	1.536940000
6	-5.123217000	-0.027045000	0.244177000
1	-3.483663000	-0.468756000	-1.125062000
1	-5.904182000	-0.280699000	-0.481687000
1	-6.526980000	0.458239000	1.822330000
1	-2.339755000	0.847808000	2.835293000
1	-4.744146000	1.017245000	3.481369000



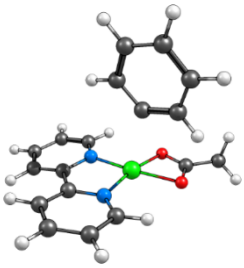
39
Aryl Carboxylate Triplet 2.9 Å Ni–C distance

C	4.708041113	0.273931660	-0.098425746
C	3.891006879	1.405125617	-0.037857388
C	4.113807696	-0.997497697	-0.060888739
C	2.726488977	-1.090200246	0.030970616
N	1.929074581	0.000000000	0.106257614
C	2.502416755	1.246809062	0.071940062
C	1.519870742	2.338251388	0.161730674
N	0.222899102	1.909675908	0.026968357
C	1.822419219	3.689649516	0.376537447
H	4.328687279	2.404907755	-0.089903473
H	5.792471500	0.380621473	-0.181873970
H	4.717890851	-1.906799994	-0.100010179
H	2.201686736	-2.048734644	0.054150126
C	0.785782713	4.623034985	0.438527564
H	2.859271871	4.006438448	0.511778993
C	-0.537925845	4.177251443	0.296416270
H	1.003774662	5.680497809	0.606910791
C	-0.775970629	2.818898859	0.103151370
H	-1.377716895	4.874518527	0.337971709
H	-1.783537045	2.409801850	-0.002010183
Ni	0.000000000	0.000000000	0.000000000
C	-0.555032749	0.170577451	2.825112220
O	-0.486998438	-1.939189324	-0.332493792
C	-1.715917447	-1.583732965	-0.410250161
O	-2.013441084	-0.342798596	-0.316840067
C	-2.796047587	-2.624592073	-0.572186231
H	-2.437849693	-3.462764235	-1.185590268
H	-3.700336153	-2.184850000	-1.012865558
H	-3.056458522	-3.025678787	0.421008082
C	-1.910528960	0.230468112	3.128456223
C	0.426574474	0.203413500	3.807886826
C	0.033540049	0.303608631	5.156830732
C	-1.326691508	0.367684499	5.487963572
C	-2.298535592	0.330643026	4.478601091
H	-2.666260717	0.194662096	2.336741263
H	-3.362432114	0.377333642	4.738487376
H	-1.630334943	0.444548095	6.536771882
H	1.491328250	0.150192609	3.554823550
H	0.793460341	0.329628278	5.946468854



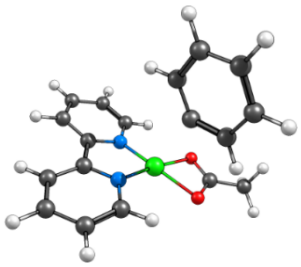
39
Aryl Carboxylate RKS 3.1 Å Ni–C distance

6	-4.619758000	0.605388000	-0.117922000
6	-4.031447000	-0.655821000	-0.188015000
6	-3.789592000	1.745195000	-0.096700000
6	-2.411105000	1.579244000	-0.148861000
7	-1.827577000	0.358106000	-0.255352000
6	-2.634007000	-0.767745000	-0.260532000
6	-1.863336000	-1.998532000	-0.333645000
7	-0.518763000	-1.794315000	-0.081858000
6	-2.355936000	-3.282758000	-0.618016000
1	-4.648607000	-1.557591000	-0.162650000
1	-5.706371000	0.706564000	-0.062780000
1	-4.211344000	2.751591000	-0.047859000
1	-1.715576000	2.421738000	-0.125777000
6	-1.481886000	-4.366584000	-0.643339000
1	-3.417237000	-3.420415000	-0.839597000
6	-0.111892000	-4.144608000	-0.398234000
1	-1.853037000	-5.370817000	-0.862167000
6	0.327118000	-2.852330000	-0.135333000
1	0.604914000	-4.968463000	-0.398996000
1	1.374753000	-2.617468000	0.063810000
28	0.000000000	0.000000000	0.000000000
6	0.540181000	-0.773187000	2.997753000
8	0.779251000	1.799592000	0.112648000
6	1.950554000	1.271857000	0.085397000
8	2.027061000	0.000000000	-0.030295000
6	3.179691000	2.126783000	0.224800000
1	3.024041000	3.105668000	-0.249101000
1	4.053711000	1.624522000	-0.210124000
1	3.376993000	2.300537000	1.295258000
6	1.872979000	-1.027322000	3.285811000
6	-0.469986000	-0.831069000	3.944907000
6	-0.120624000	-1.163142000	5.269002000
6	1.216674000	-1.425857000	5.596723000
6	2.212446000	-1.359427000	4.612522000
1	2.642589000	-0.970185000	2.509473000
1	3.257034000	-1.565212000	4.872565000
1	1.484485000	-1.683713000	6.626008000
1	-1.514384000	-0.625078000	3.686752000
1	-0.896633000	-1.215647000	6.041076000



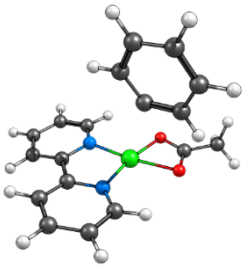
39
Aryl Carboxylate Triplet 3.1 Å Ni–C distance

C	4.668911097	0.278251076	-0.429837405
C	3.858299803	1.408116680	-0.302925651
C	4.080818908	-0.994433766	-0.335491836
C	2.707940989	-1.089380945	-0.121376855
N	1.917119386	0.000000000	0.026456249
C	2.485671567	1.249532558	-0.066792678
C	1.511182616	2.333989366	0.099864848
N	0.208817057	1.900299921	0.016192761
C	1.817254965	3.681636413	0.333117036
H	4.284936440	2.409057082	-0.404644737
H	5.741194246	0.385298437	-0.611473500
H	4.680643299	-1.903287410	-0.422230115
H	2.189551330	-2.048901676	-0.049368054
C	0.781075129	4.607311878	0.468015400
H	2.858637338	3.998291998	0.429577106
C	-0.546923935	4.156663945	0.382754841
H	1.002011876	5.661647464	0.651477712
C	-0.788838137	2.802344362	0.170175671
H	-1.386793431	4.848106461	0.481052541
H	-1.798831417	2.390690178	0.106492804
Ni	0.000000000	0.000000000	0.000000000
C	-0.494358589	0.204258580	3.008654402
O	-0.496911519	-1.938756313	-0.253165834
C	-1.729583400	-1.588666604	-0.238780212
O	-2.018169879	-0.345251393	-0.139118418
C	-2.817382683	-2.630884557	-0.302242405
H	-2.502908618	-3.481620780	-0.922173744
H	-3.750061797	-2.198620291	-0.687810204
H	-3.008515956	-3.010862936	0.714699689
C	-1.847151113	0.254104628	3.315733664
C	0.501541073	0.252216291	3.973282430
C	0.119308393	0.359045062	5.325053451
C	-1.238693167	0.413309488	5.668064735
C	-2.221311587	0.360636224	4.669589742
H	-2.606812819	0.207140774	2.528624495
H	-3.282459534	0.400718981	4.940946701
H	-1.532455929	0.495002918	6.719177940
H	1.562923661	0.206285415	3.706425883
H	0.885521482	0.398109997	6.107812395



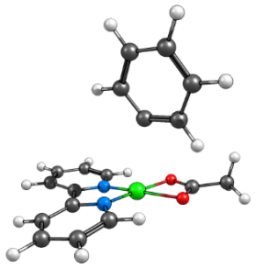
39
Aryl Carboxylate RKS 3.3 Å Ni–C distance

6	-4.625000000	0.562765000	0.051717000
6	-4.026528000	-0.695595000	0.063932000
6	-3.807704000	1.705940000	-0.067091000
6	-2.431214000	1.545359000	-0.170083000
7	-1.839731000	0.324054000	-0.197669000
6	-2.632969000	-0.803844000	-0.066449000
6	-1.853321000	-2.030858000	-0.072076000
7	-0.501013000	-1.797194000	0.106991000
6	-2.344375000	-3.336801000	-0.231943000
1	-4.631521000	-1.595976000	0.198370000
1	-5.708851000	0.660698000	0.150401000
1	-4.237910000	2.709737000	-0.087204000
1	-1.745011000	2.391666000	-0.254276000
6	-1.461853000	-4.413931000	-0.206554000
1	-3.412391000	-3.498337000	-0.398728000
6	-0.085037000	-4.163832000	-0.038981000
1	-1.831920000	-5.434896000	-0.328310000
6	0.351847000	-2.851583000	0.099761000
1	0.639190000	-4.980452000	-0.003364000
1	1.405133000	-2.595135000	0.232760000
28	0.000000000	0.000000000	0.000000000
6	0.760439000	-0.600966000	3.169206000
8	0.775545000	1.807903000	-0.072512000
6	1.945155000	1.278084000	-0.074996000
8	2.020293000	0.000000000	-0.069412000
6	3.178260000	2.138763000	-0.048674000
1	3.009298000	3.071037000	-0.604739000
1	4.039255000	1.596688000	-0.461291000
1	3.407188000	2.408010000	0.995416000
6	2.120674000	-0.803808000	3.339963000
6	-0.160225000	-0.619634000	4.203261000
6	0.320216000	-0.858469000	5.506518000
6	1.689377000	-1.068597000	5.722295000
6	2.588986000	-1.042346000	4.647757000
1	2.811113000	-0.777914000	2.491364000
1	3.658361000	-1.206794000	4.821627000
1	2.057994000	-1.253754000	6.735843000
1	-1.228890000	-0.454642000	4.029779000
1	-0.379286000	-0.879596000	6.349722000



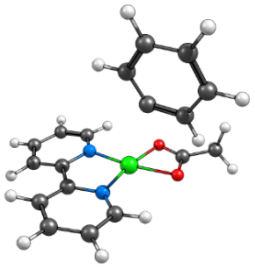
39
Aryl Carboxylate Triplet 3.3 Å Ni–C distance

C	4.670889835	0.222555601	-0.200245452
C	3.864546315	1.361288400	-0.230724850
C	4.066648314	-1.033067011	-0.006783851
C	2.685193482	-1.101961081	0.147290364
N	1.895501881	0.000000000	0.149667621
C	2.480413805	1.233892890	-0.046532731
C	1.506805874	2.326019874	-0.042924389
N	0.208933885	1.880662566	-0.176769225
C	1.798293215	3.691091766	0.088091007
H	4.302145813	2.345242975	-0.417543605
H	5.751543759	0.306191878	-0.339428407
H	4.662250857	-1.948048644	0.031174123
H	2.156920610	-2.047939864	0.290666549
C	0.758249907	4.621143914	0.068686326
H	2.831740487	4.017927295	0.227876834
C	-0.563705313	4.159055750	-0.061661156
H	0.968676985	5.688624515	0.170178520
C	-0.794684526	2.790909838	-0.165517736
H	-1.406344432	4.853746676	-0.084105371
H	-1.799592215	2.372184108	-0.257980841
Ni	0.000000000	0.000000000	0.000000000
C	-0.827411399	0.598328092	3.152074776
O	-0.499113179	-1.949105488	-0.012773436
C	-1.727920785	-1.591883589	-0.063627676
O	-2.000884357	-0.340858548	-0.123879601
C	-2.827709608	-2.621033818	-0.017483553
H	-2.505819670	-3.553512585	-0.500716807
H	-3.740205694	-2.237412250	-0.492694577
H	-3.059621512	-2.851063096	1.035332109
C	-2.209503257	0.656477212	3.231298769
C	0.018644803	0.774233852	4.234045867
C	-0.566838328	1.031362824	5.490073602
C	-1.961337802	1.100622365	5.613416917
C	-2.782648931	0.914306839	4.492566681
H	-2.836553314	0.504560775	2.347092021
H	-3.872396001	0.967307947	4.594460334
H	-2.411351552	1.299581198	6.590871428
H	1.107418877	0.716884875	4.132496251
H	0.071249047	1.175780298	6.369103775



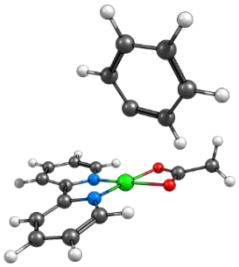
39
Aryl Carboxylate RKS 3.5 Å Ni–C distance

6	4.645576000	0.259662000	0.245650000
6	3.836933000	1.393445000	0.192582000
6	4.046048000	-1.011518000	0.131735000
6	2.668364000	-1.097119000	-0.030833000
7	1.874724000	0.000000000	-0.121961000
6	2.453228000	1.252334000	0.003080000
6	1.473252000	2.323796000	-0.078208000
7	0.175899000	1.863544000	0.067638000
6	1.738063000	3.687832000	-0.280988000
1	4.269021000	2.389149000	0.321947000
1	5.724365000	0.355895000	0.390820000
1	4.644947000	-1.924535000	0.161045000
1	2.144672000	-2.052642000	-0.114572000
6	0.682507000	4.595347000	-0.332024000
1	2.767905000	4.025542000	-0.422391000
6	-0.636128000	4.114930000	-0.199010000
1	0.875111000	5.659686000	-0.487624000
6	-0.844726000	2.752876000	-0.017008000
1	-1.491712000	4.793281000	-0.223386000
1	-1.842679000	2.322882000	0.091571000
28	0.000000000	0.000000000	0.000000000
6	-1.099418000	0.670088000	3.239062000
8	-0.452621000	-1.926063000	-0.027049000
6	-1.693237000	-1.600773000	-0.046667000
8	-1.983967000	-0.353197000	-0.072708000
6	-2.766216000	-2.654478000	-0.003886000
1	-2.432082000	-3.565642000	-0.518470000
1	-3.696306000	-2.280413000	-0.451796000
1	-2.971401000	-2.917887000	1.046631000
6	-2.480650000	0.575247000	3.247163000
6	-0.327254000	0.944646000	4.353675000
6	-0.997894000	1.139214000	5.578267000
6	-2.395773000	1.052682000	5.634600000
6	-3.137684000	0.772646000	4.478469000
1	-3.042237000	0.354281000	2.334376000
1	-4.230194000	0.705980000	4.528515000
1	-2.911218000	1.204491000	6.587778000
1	0.764540000	1.010726000	4.302403000
1	-0.422881000	1.358268000	6.484817000



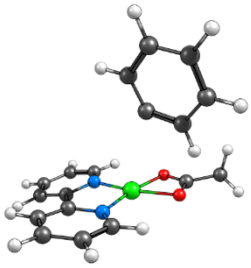
39
Aryl Carboxylate Triplet 3.6 Å Ni–C distance

C	4.652768551	0.248397312	-0.340308909
C	3.844348193	1.384346398	-0.291098731
C	4.056010899	-1.017748235	-0.188400369
C	2.680981863	-1.098426156	0.006559091
N	1.889506431	0.000000000	0.090243210
C	2.466676537	1.245415306	-0.068265333
C	1.490686728	2.328463802	0.015191924
N	0.190431415	1.879190971	-0.108025901
C	1.774946151	3.688674627	0.204214770
H	4.273535274	2.377472573	-0.446862566
H	5.728179127	0.341563962	-0.510518556
H	4.653805962	-1.931776864	-0.212841503
H	2.159462256	-2.052004881	0.121377657
C	0.728959238	4.610104282	0.255784325
H	2.809627417	4.016166868	0.333744938
C	-0.593868297	4.143920900	0.138280876
H	0.934752869	5.673240262	0.402467468
C	-0.818671440	2.780963536	-0.024417271
H	-1.441457156	4.832247736	0.169085135
H	-1.822806747	2.359333431	-0.111945636
Ni	0.000000000	0.000000000	0.000000000
C	-0.958525837	0.555630482	3.394605993
O	-0.493288420	-1.946969499	-0.041814946
C	-1.722734606	-1.591566987	-0.024026769
O	-1.995573962	-0.337878068	-0.025062245
C	-2.821231450	-2.621045711	0.031076683
H	-2.513744385	-3.542616875	-0.481278729
H	-3.745970422	-2.226694062	-0.410734826
H	-3.025829650	-2.873278137	1.084505712
C	-2.339967841	0.540560425	3.315709519
C	-0.236297733	0.748748954	4.557901817
C	-0.967026090	0.946824568	5.747253016
C	-2.368478467	0.942022744	5.719262229
C	-3.055379404	0.740333254	4.513806999
H	-2.855978941	0.378154408	2.364567865
H	-4.150868868	0.736367142	4.499061578
H	-2.930262786	1.095705050	6.645529823
H	0.858377461	0.749729106	4.570890777
H	-0.435222239	1.103616092	6.692116013



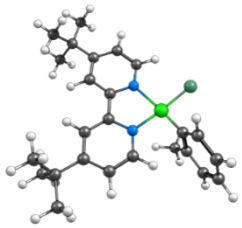
39
Aryl Carboxylate RKS 3.9 Å Ni–C distance

6	4.649472000	0.268464000	-0.147066000
6	3.835596000	1.400251000	-0.153230000
6	4.045524000	-1.004537000	-0.194105000
6	2.659207000	-1.094012000	-0.246026000
7	1.857052000	0.000000000	-0.291001000
6	2.442088000	1.254015000	-0.231427000
6	1.456494000	2.324626000	-0.254932000
7	0.177646000	1.869764000	0.020589000
6	1.701443000	3.679904000	-0.525362000
1	4.273426000	2.398640000	-0.072418000
1	5.736094000	0.368317000	-0.088445000
1	4.646862000	-1.916519000	-0.199126000
1	2.133501000	-2.051757000	-0.273989000
6	0.644967000	4.588719000	-0.511225000
1	2.714300000	4.009963000	-0.770408000
6	-0.656025000	4.115144000	-0.247927000
1	0.822126000	5.647069000	-0.717837000
6	-0.846683000	2.759447000	-0.006248000
1	-1.510790000	4.794559000	-0.218285000
1	-1.832072000	2.335790000	0.199934000
28	0.000000000	0.000000000	0.000000000
6	-1.182382000	0.981031000	3.631192000
8	-0.465793000	-1.940456000	0.062378000
6	-1.691780000	-1.600820000	0.202940000
8	-1.974950000	-0.348972000	0.207517000
6	-2.765113000	-2.639904000	0.391508000
1	-2.480509000	-3.581671000	-0.096284000
1	-3.726159000	-2.280779000	-0.000593000
1	-2.890310000	-2.840109000	1.468322000
6	-2.521353000	0.749570000	3.378649000
6	-0.653448000	1.399147000	4.836718000
6	-1.562529000	1.605922000	5.894759000
6	-2.932907000	1.387498000	5.695937000
6	-3.414049000	0.962691000	4.449508000
1	-2.871093000	0.415812000	2.397245000
1	-4.486219000	0.793757000	4.301899000
1	-3.632772000	1.549742000	6.521015000
1	0.418672000	1.566719000	4.979788000
1	-1.192502000	1.937493000	6.870871000



39
Aryl Carboxylate Triplet 3.9 Å Ni–C distance

C	4.642398146	0.223090009	-0.430936682
C	3.836647745	1.361508339	-0.420590304
C	4.045651306	-1.034121482	-0.212243978
C	2.674287626	-1.102935541	0.008578636
N	1.885324276	0.000000000	0.056940036
C	2.462197041	1.236710429	-0.169357432
C	1.488669968	2.321687944	-0.121323889
N	0.185833521	1.865589278	-0.206406549
C	1.772605490	3.689894391	0.001236675
H	4.264288314	2.345547151	-0.629578526
H	5.714997354	0.305791571	-0.622910380
H	4.641509833	-1.949727903	-0.204596740
H	2.153616179	-2.049356902	0.174928284
C	0.726359862	4.611826943	0.023198699
H	2.808433847	4.023808159	0.102651312
C	-0.598101136	4.139389829	-0.054772135
H	0.932472402	5.680840466	0.117328490
C	-0.823406409	2.770491855	-0.149793159
H	-1.446069576	4.827900122	-0.046222020
H	-1.828160829	2.344870187	-0.204963158
Ni	0.000000000	0.000000000	0.000000000
C	-1.291392700	0.874636817	3.589988220
O	-0.493454408	-1.944005330	0.087694750
C	-1.721415157	-1.585688514	0.112105687
O	-1.992777151	-0.333114310	0.046365205
C	-2.821570882	-2.605892205	0.248266375
H	-2.511805746	-3.568997173	-0.178822119
H	-3.741739997	-2.250589874	-0.234753823
H	-3.038031296	-2.762939061	1.317753686
C	-2.623713155	0.771037899	3.237858390
C	-0.814425609	1.205534585	4.843611682
C	-1.773007898	1.459612783	5.845945433
C	-3.139615569	1.370743696	5.547249787
C	-3.566163855	1.029679019	4.255998107
H	-2.948715122	0.501630599	2.227968346
H	-4.636252121	0.961744571	4.031305374
H	-3.879474331	1.568494630	6.328607838
H	0.255696618	1.271112725	5.063938275
H	-1.444695546	1.725626454	6.856478643



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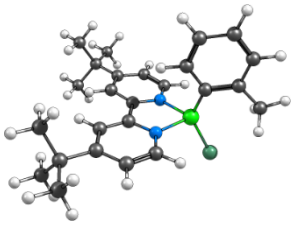
Aryl Chloride RKS 1.6 Å Ni–C distance

Ni	-0.00009519129503	-0.00016310960331	-0.00000559617899
C	-2.43145763719745	1.41863184932317	0.01090148403728
C	-2.79218288280194	-0.87955592552047	0.08630258146515
C	-3.80984294345521	1.64694475770289	0.04767053979983
C	-4.17205284067798	-0.70011716425471	0.12147756022553
H	-2.35431376070488	-1.87764533291615	0.10513647032714
C	-4.73205874349013	0.58928814213786	0.10340561047272
H	-4.16752313526241	2.67855463662640	0.03529119683099
H	-4.79821914686812	-1.59238178530806	0.16475167365093
C	-1.42168697925816	2.48616110132030	-0.04585755681574
C	-1.70183475889974	3.85653736721692	-0.10297702777062
C	-0.66374388074989	4.80317804644603	-0.14851345937532
H	-2.74145120316643	4.19012588392263	-0.11482155355137
C	0.85965547017024	2.91122269938295	-0.07769745091348
C	0.64473960934390	4.28895882008757	-0.13279348990369
H	1.86328949382268	2.47703457827532	-0.06691450042889
H	1.51428075555177	4.94679422047674	-0.16408375840904
C	-0.00009559771166	-1.60016300372786	-0.00058392471423
C	-0.12221385815623	-2.34862869860776	-1.21119290609299
C	-0.02330951103334	-2.31748115982147	1.22218853849375
C	-0.30809684522590	-3.74052661513035	-1.14825106454678
C	-0.21094514897102	-3.70634074695283	1.26135279573674
C	-0.36716174035979	-4.42613516656720	0.07198310463159
H	-0.40256666639296	-4.29987850124645	-2.08708388831807
H	-0.22554242021213	-4.22238145923508	2.22753073214437
Cl	2.16958162235690	-0.00533808857864	0.00036995323203
N	-1.90267773774330	0.14473981132651	0.02915552834309
N	-0.14244973411924	2.01368476715378	-0.03497032567136
H	0.11914945114475	-1.78042729741296	2.16632049421215
H	-0.51105147672642	-5.51066297610340	0.08947739439966
C	-6.24241363233700	0.86328281810150	0.14350559355303
C	-0.98104397731519	6.30557436382766	-0.21179879772830
C	-6.65310736158452	1.64611110658773	-1.12863322216664
H	-6.42777959660785	1.07086453742722	-2.04044926365421
H	-6.13272552705455	2.61358388823135	-1.20557741884427
H	-7.73580092532322	1.85235855088687	-1.11541877387570
C	-6.57463823214545	1.70848102526103	1.39859199209978
H	-6.05188683452903	2.67770441439613	1.39535070233297
H	-6.29228040572331	1.17853194678159	2.32189153445182
H	-7.65641088186042	1.91539837519315	1.44236327985018
C	-7.06375736480908	-0.43956315058676	0.20114818309673
H	-6.83797349226754	-1.03118155574553	1.10270746584361
H	-6.89182825981827	-1.07627899792377	-0.68138920814884
H	-8.13831067456971	-0.20010631938629	0.22758389708582
C	-1.81257129857104	6.59738874071479	-1.48578652492613
H	-2.76676946792446	6.04791216281599	-1.49316369714698
H	-1.25829245052479	6.31898698793331	-2.39591709347576
H	-2.04854575641794	7.67226980241051	-1.54690519961388
C	-1.79830773566687	6.70640281992162	1.04159626203189
H	-1.23344728030796	6.50752878855141	1.96597062913101
H	-2.75181103054882	6.15950145412295	1.10713803466336
H	-2.03463666097684	7.78254616573156	1.01245904754398
C	0.29694692164003	7.16583755620177	-0.25627521722561
H	0.91210110492095	6.94734411777658	-1.14371175771337
H	0.92194273492345	7.02540584573261	0.64004590327677
H	0.02472404851955	8.23192113195889	-0.30135425892844
C	-0.02321235292252	-1.66271102502664	-2.55757282274326
H	0.95405575968638	-1.16489895884798	-2.67051430214195
H	-0.79216515308397	-0.88021816194102	-2.68457314132458
H	-0.13755440471084	-2.38009037652062	-3.38597216361538



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Aryl Chloride Triplet 1.6 Å Ni–C distance

Ni	-0.00001814851899	0.00024948128067	0.00016081043439
C	2.41995753548792	1.23118368271145	-0.83123144085451
C	2.72318443713820	-1.06426620841106	-0.51181974512951
C	3.78669336670465	1.38424319001933	-1.10624220215431
C	4.08144323859412	-0.96887805059321	-0.79701034713428
H	2.25537413550443	-2.02087875664166	-0.26586902783566
C	4.65691523790333	0.28423741190075	-1.10031750859210
H	4.17144864340233	2.38112035823472	-1.33331715853182
H	4.68070967563701	-1.87983332511796	-0.77898330925812
C	1.42511935719793	2.31126840525159	-0.83103341905930
C	1.68965401396902	3.66083304569517	-1.10620004557063
C	0.66472681773066	4.61835012135148	-1.09997884185452
H	2.71463552836385	3.96247971488487	-1.33381310645378
C	-0.83759823043493	2.80176560168237	-0.51078499098607
C	-0.63122565212074	4.14763052019311	-0.79599325010892
H	-1.82928539195277	2.41398423526266	-0.26455829225082
H	-1.48996997283918	4.81956246443707	-0.77769292888122
C	-0.00006088900496	-0.00017432515758	1.60016075158076
C	-0.90679192783471	-0.83531661143128	2.34877100417521
C	0.88107234251476	0.81100793382467	2.36910616821349
C	-0.87440810973496	-0.80581789680791	3.75708084445163
C	0.89737383101644	0.82569883925765	3.76596690032336
C	0.00876463373093	0.00731579354513	4.47182346725578
H	-1.57317871109478	-1.44945664361412	4.30458082312950
H	1.60171250797638	1.47411765804728	4.29854679471734
Cl	-1.21044418570149	-1.11448980214495	-1.54589838988431
N	1.89734865248229	0.00023746476285	-0.52955664390824
N	0.15555158594843	1.89137691241157	-0.52898120920058
H	1.59202033119444	1.46573239857858	1.84863364019347
H	0.00138983942653	0.00027213230947	5.56611428530248
C	6.15101468615610	0.46948007169922	-1.41196794250195
C	0.97173945626243	6.09216036216715	-1.41214862876050
C	6.30602433441343	1.06749472148547	-2.83250359176511
H	5.86859018024529	0.40326508007517	-3.59435934215682
H	5.81663309060162	2.04964427075511	-2.92403342295449
H	7.37292149440754	1.20509961897815	-3.07282950710634
C	6.77235539750064	1.43667419332219	-0.37366800631592
H	6.29487093048741	2.42870541604546	-0.39464701222559
H	6.67488014777875	1.03950694129191	0.64901844433448
H	7.84514993263563	1.58052024099371	-0.58209189010635
C	6.92343517563573	-0.86332171649925	-1.35848139249800
H	6.87769043924177	-1.32874681956528	-0.36087509932960
H	6.54736284900771	-1.58968791017796	-2.09661672119393
H	7.98577103263421	-0.68534073307491	-1.58747320338789
C	1.57882677251139	6.19733496395498	-2.83338846740993
H	2.51733565450395	5.62889504119388	-2.92595486630029
H	0.88001233225945	5.81589540720696	-3.59440212555015
H	1.80336981995968	7.24928305181999	-3.07410354197176
C	1.98795032500450	6.63201628368602	-0.37510950463238
H	1.58530233440629	6.56771715623104	0.64805619922923
H	2.93731783031230	6.07452682144358	-0.39711789001919
H	2.21931190588506	7.68930918549521	-0.58397820185112
C	-0.29297780067161	6.97153347294900	-1.35737628951425
H	-1.04863261453991	6.65631779439354	-2.09460527928443
H	-0.75945320979732	6.96438540690526	-0.35923480079919
H	-0.02848829494889	8.01558745897346	-1.58686492836864
C	-1.90939070172314	-1.75870668442517	1.68554935274587
H	-2.61254087206837	-1.21656051298995	1.03430570972460
H	-1.42677019618432	-2.50409449124866	1.03444514537944
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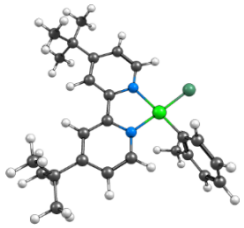

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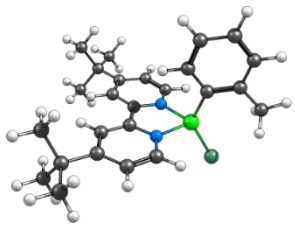
Aryl Chloride RKS 1.8 Å Ni–C distance

Ni	-0.00002879528857	-0.00005290828175	0.00010736647551
C	-2.39732076031478	1.41830539624174	0.01579002381288
C	-2.78090063746139	-0.87846025090131	-0.00294303125105
C	-3.77308044035989	1.66049095560419	0.02233782756931
C	-4.15928055119254	-0.68396970490465	0.00124695488195
H	-2.35259623868496	-1.88058167322444	-0.00903770104575
C	-4.70672148167320	0.61117873413428	0.01472863461740
H	-4.11927543741318	2.69621445380687	0.03411271391587
H	-4.79513731565527	-1.57043133400755	-0.00559127275680
C	-1.37135685819065	2.46868182264374	0.02268378669924
C	-1.62172029279259	3.84504172596520	0.03234581561764
C	-0.56454975649523	4.77155620040930	0.04043904910092
H	-2.65494447684533	4.19846580379019	0.03314418973405
C	0.92161313887808	2.84732882005648	0.02829000412507
C	0.73293989886166	4.22935955743009	0.03852919547093
H	1.91616269847368	2.39295319142558	0.02569438357458
H	1.61605274152883	4.86961657846533	0.04458823289850
C	-0.00000964811992	-1.80005288154110	-0.00019906341853
C	-0.06110545865039	-2.54045624138021	-1.20741773904902
C	-0.06117034121954	-2.49056479802610	1.22511725899322
C	-0.21098306236977	-3.93834062450885	-1.14476842806771
C	-0.20829792839914	-3.88544966896525	1.27061124077580
C	-0.29331757066434	-4.61391842704291	0.07946585048811
H	-0.25651576931811	-4.50819413884838	-2.08068464280682
H	-0.25003231089645	-4.39763189154562	2.23785056991832
Cl	2.16490389913508	-0.08137803512117	0.00018634022254
N	-1.87907591282569	0.13781091561163	0.00315253216250
N	-0.09951922712769	1.96822219672867	0.02018076917060
H	0.02203228724412	-1.93638918476868	2.16634372430243
H	-0.40616768753580	-5.70232938152234	0.09982178453405
C	-6.21493710219446	0.89935243067356	0.02230360694704
C	-0.85048101731024	6.28131277302125	0.05120697731763
C	-6.58235106861198	1.73171251041252	-1.23149980467300
H	-6.33686151885389	1.18731101005884	-2.15695006527983
H	-6.05079299562125	2.69578348553296	-1.25884990187736
H	-7.66298942675060	1.94879296316273	-1.24096162533981
C	-6.57476385991447	1.70222752293214	1.29737263533236
H	-6.04261664092379	2.66524449355646	1.34410688475097
H	-6.32396062931439	1.13629199442869	2.20835438837251
H	-7.65526853850058	1.91922896302613	1.31827115975833
C	-7.04988947929149	-0.39606831784487	0.00959942734061
H	-6.85513230686808	-1.02229917381229	0.89488840648992
H	-6.85910738700478	-1.00211332489085	-0.89049536578464
H	-8.12248105306619	-0.14659596355366	0.01486976275361
C	-1.66770603363355	6.65427989105091	-1.21078750322422
H	-2.63285276018884	6.12565838395015	-1.25093429919195
H	-1.11339827906562	6.41055269271002	-2.13079893862843
H	-1.88139515563435	7.73552815748045	-1.21891386688970
C	-1.66728934498775	6.63574565180392	1.31882933393902
H	-1.11260499313612	6.37870800825399	2.23497907670478
H	-2.63226450216062	6.10627707439292	1.35157444874394
H	-1.88118880003508	7.71672492750265	1.34282239650962
C	0.44530513489964	7.11571120490022	0.05700252743125
H	1.06162734976338	6.92911942907415	-0.83690237886884
H	1.06136514632763	6.91734223103630	0.94853749296922
H	0.19558157445829	8.18822231900452	0.06411301320013
C	0.06331837431322	-1.85007190304765	-2.54799550253367
H	1.03417863650046	-1.33430881552447	-2.62906512263754
H	-0.71548719806888	-1.08054467895890	-2.68974203373523
H	-0.01566962375261	-2.56495128305577	-3.38244373656241



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Aryl Chloride Triplet 1.8 Å Ni–C distance

Ni	-0.00006183850344	0.00024711447285	0.00001133050884
C	2.44024470402626	1.22355589042359	-0.77226673773056
C	2.73111674208350	-1.06725417322856	-0.43137553311302
C	3.80522826954629	1.36823504012220	-1.05399847346495
C	4.09132205694173	-0.98072511921332	-0.71443326551062
H	2.25948909808227	-2.01913729514657	-0.17459192278445
C	4.67155071593231	0.26382671534331	-1.03548247047599
H	4.19403299123585	2.36049218707771	-1.29365741824276
H	4.68742999671712	-1.89335498080987	-0.68040212045696
C	1.45056142817960	2.31271774305159	-0.77213352901019
C	1.72487818203026	3.65766524009005	-1.05380589597672
C	0.70827169565455	4.62552597535164	-1.03495876113198
H	2.74968772338891	3.94990252903756	-1.29374435637438
C	-0.80190739572664	2.82101075957172	-0.43067369978277
C	-0.58592115942905	4.16677626343574	-0.71357691668393
H	-1.79443289654528	2.44243112992562	-0.17372693622958
H	-1.43744898788985	4.84729094122924	-0.67926272421595
C	-0.00014909714491	-0.00005227196299	1.80001130286397
C	-0.89659980639900	-0.81475297161792	2.55438334639711
C	0.89694504740106	0.81493890478811	2.52539741699421
C	-0.85172438572350	-0.77411889272742	3.96202535223915
C	0.93306115482571	0.84756623855019	3.92513270088251
C	0.04874224784062	0.04400576703272	4.65156404827941
H	-1.54661970554407	-1.40564741437365	4.52844441331419
H	1.64805008168858	1.49712146926642	4.44209532754983
Cl	-1.24546001245444	-1.13177326274131	-1.46176173818456
N	1.90995550153085	0.00022630377906	-0.46086236743909
N	0.18223971222379	1.90163158026701	-0.46053751640797
H	1.60289430321331	1.45645802022791	1.98206344186459
H	0.05745705097425	0.05178391043647	5.74615847090916
C	6.16560132737820	0.43884367019327	-1.35211204926111
C	1.02512852695281	6.09606223890002	-1.35162916794198
C	6.31988369259030	1.01577498454604	-2.78144889591104
H	5.87917964212969	0.34201448677489	-3.53298471156927
H	5.83374763899965	1.99820087935146	-2.88646680076304
H	7.38681349256427	1.14628042840080	-3.02531703100417
C	6.79187468316309	1.41877136531359	-0.32876959823823
H	6.31831414682301	2.41229747340861	-0.36346013990230
H	6.69461047591251	1.03691761719856	0.69971771556380
H	7.86479355173248	1.55541565546284	-0.54101944145874
C	6.93296848884858	-0.89596731974394	-1.28056482286522
H	6.88748397075661	-1.34656256936111	-0.27617571303283
H	6.55284428342061	-1.63159613526717	-2.00736987914345
H	7.99549558165485	-0.72535246481566	-1.51404814658409
C	1.61328651860416	6.19459686204678	-2.78129659012769
H	2.54463868485065	5.61671999967429	-2.88693521182939
H	0.89999742567418	5.82046819927039	-3.53244858915214
H	1.84513051979310	7.24416711931180	-3.02519959701200
C	2.06112950990159	6.62563194909790	-0.32891588566016
H	1.67241529118712	6.56523174983047	0.69982532475228
H	3.00477989607566	6.05921167317627	-0.36431507150456
H	2.29962722186481	7.68058616600918	-0.54121105595587
C	-0.23008389756955	6.98760318051929	-1.27923961564910
H	-0.99915949700804	6.67965508583302	-2.00558654188438
H	-0.68232817105357	6.98538840977913	-0.27456127560633
H	0.04129838307982	8.02893378242890	-1.51284372387608
C	-1.90380424051790	-1.73019249815296	1.88906086606668
H	-2.59935335355294	-1.17838260668677	1.23721234779066
H	-1.42067635403350	-2.47542102589422	1.23759662483967
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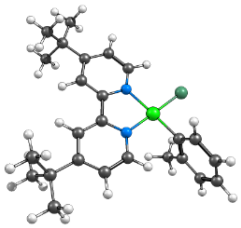

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Aryl Chloride RKS Fully Optimized

Ni	1.25914263866544	-1.29757372487669	-0.14112525437629
C	-0.53174202130060	0.82236263138977	-0.05276765965357
C	1.66882229381741	1.58482149937974	-0.09475688098736
C	-1.00041811644866	2.13755601376627	-0.01594938200899
C	1.24638321690200	2.91079811341753	-0.05677506044416
H	2.72774103352657	1.32971435780501	-0.13107327951978
C	-0.12169966702071	3.23352499929650	-0.01636271773084
H	-2.07925406113239	2.30512352686027	0.01374107432126
H	2.01391709480731	3.68608976935289	-0.06033122930693
C	-1.39263143480114	-0.36642486475297	-0.05295364225741
C	-2.79074638678948	-0.35569668576642	-0.01574421366813
C	-3.52334485816867	-1.55557176679547	-0.02061400682915
H	-3.31453146242078	0.60196657867422	0.01773258177511
C	-1.37443268109171	-2.69117663415023	-0.10054220131032
C	-2.76780579930842	-2.74084937248017	-0.06487415953652
H	-0.75731215719097	-3.59314116075665	-0.13480541898368
H	-3.24785264820125	-3.72032346798859	-0.07211723022273
C	3.12167799417186	-0.98525023074852	-0.21289635542658
C	3.88713966266663	-0.84006451036810	0.96707410642455
C	3.73442935142503	-0.78892449449916	-1.46139520337966
C	5.24206114585184	-0.47418450938750	0.85633735540310
C	5.08769209787184	-0.42730317983252	-1.55596047625282
C	5.84336057278074	-0.26077583456522	-0.39062653672574
H	5.83796598690090	-0.36284189962233	1.77020551289907
H	5.54677431674462	-0.28304535751910	-2.53982302287140
Cl	1.72076309007112	-3.41224871316937	-0.19215085325278
N	0.81734183325104	0.52585068203240	-0.09374530448884
N	-0.68231175198931	-1.53458309165407	-0.09506518765389
H	3.15763893991219	-0.93357642425723	-2.38121911477150
H	6.89988598270750	0.01894601327378	-0.44922887060878
C	-0.65734502626263	4.67204552570972	0.02450604903262
C	-5.05921626916135	-1.53232244816780	0.02036859476526
C	-1.49469553694754	4.86914370827726	1.31285159728213
H	-0.88484449529059	4.69914097904711	2.21411461062482
H	-2.35520170679103	4.18334406818115	1.35630102700777
H	-1.88824327947235	5.89779649575126	1.35739925369609
C	-1.55320168785508	4.91876094207600	-1.21503149159144
H	-2.41524944149532	4.23419170433869	-1.24560349843737
H	-0.98577866310069	4.78494194026435	-2.14948079092735
H	-1.94763424698216	5.94795307964326	-1.20086016146429
C	0.48051932323975	5.71159325100046	0.01864066976738
H	1.09909773993250	5.64243184315293	-0.89043370459579
H	1.14096453079650	5.60657776911028	0.89422305831025
H	0.05588365268223	6.72720953839913	0.04896934929135
C	-5.52387743589316	-0.81303922857806	1.31123275116574
H	-5.16680567530302	0.22757305102885	1.35733578111832
H	-5.15835532455597	-1.33312100462607	2.21066792518388
H	-6.62484696915958	-0.78800634997499	1.35671367346684
C	-5.59021531154789	-0.76660623867138	-1.21713818715370
H	-5.27289080024962	-1.25302899077683	-2.15296073101891
H	-5.23486465871328	0.27528739372898	-1.24373330169090
H	-6.69203617921610	-0.74088870301986	-1.20389692229145
C	-5.65991034716769	-2.95161252088294	0.01016972473181
H	-5.34110698622560	-3.54215257144896	0.88387603002167
H	-5.38917654798001	-3.50913605271111	-0.90064927672812
H	-6.75893994070766	-2.88927610549583	0.04085694122440
C	3.27652035100237	-1.10068026789563	2.32611105203635
H	2.91963209269041	-2.14124019976414	2.39589697590361
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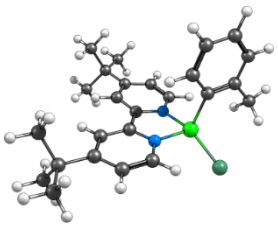
H	4.00137774553978	-0.93107637825930	3.13807883881008



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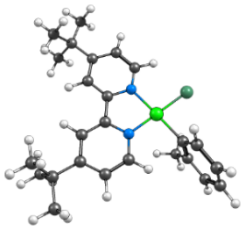
Aryl Chloride Triplet Fully Optimized

Ni	-0.23540777135903	0.31018446026536	0.13459255983897
C	2.29083220390681	1.34518716335624	-0.59101766611350
C	2.41894178782609	-0.95941701734680	-0.25254800890352
C	3.67862265222037	1.40681453530990	-0.77180375522411
C	3.79551904156790	-0.95610423959661	-0.44849690163390
H	1.88527657974779	-1.88410687668948	-0.01892292753061
C	4.47396337289971	0.25251156758757	-0.71426446802925
H	4.14289137231177	2.37915759083879	-0.95208714706508
H	4.32971735121659	-1.90484279452097	-0.38444273600487
C	1.38209920467270	2.49849260938635	-0.63322982142253
C	1.74031281367590	3.80991529531082	-0.97339327091469
C	0.79120954430733	4.84434481210330	-0.96910637049882
H	2.77527271715399	4.02080757817278	-1.25200158271982
C	-0.83262578609093	3.16770319808593	-0.28797819363013
C	-0.52576622945333	4.48674680618784	-0.60996933761666
H	-1.84507684647038	2.85345034800304	-0.02328745335014
H	-1.32674288603741	5.22628783262283	-0.58093048412576
C	-0.00426178361110	0.03714090469346	2.04627432835091
C	-0.34056591998319	-1.20678524282082	2.63175418766855
C	0.50687966242832	1.05698112348022	2.86358650884769
C	-0.16578561154844	-1.37757882343230	4.01850902790557
C	0.66858535963986	0.87839459568668	4.24660042341246
C	0.32968658980627	-0.34762781558011	4.82664292113218
H	-0.42894601153568	-2.34097653800853	4.47196327789024
H	1.05973915161548	1.69510656527290	4.86323368198969
Cl	-2.29838784081982	-0.05305797102294	-0.53980969461748
N	1.65736749083207	0.15399977748992	-0.32945459299786
N	0.09150037144065	2.18567235375279	-0.29926766590483
H	0.78326605897266	2.02334074500650	2.42577268559753
H	0.45344245570863	-0.50655411562674	5.90253052610902
C	5.99500307552973	0.33854120901088	-0.91730410703323
C	1.19915686901311	6.27752324448861	-1.34738072779932
C	6.29212938093399	0.93777174673205	-2.31444038628769
H	5.86971382619168	0.31055726178903	-3.11532007825794
H	5.87572618815676	1.95086322895679	-2.42745052436924
H	7.38036832994346	1.00736067340604	-2.47519715448153
C	6.60372146201723	1.25167435246038	0.17613215913840
H	6.19728418621283	2.27421413254278	0.13429841238705
H	6.40471099864452	0.85357102548860	1.18349088805518
H	7.69616942960706	1.32315793809600	0.04739670325123
C	6.66971524315749	-1.04438094113250	-0.82787951857095
H	6.52602650002621	-1.51214043038746	0.15922973123088
H	6.29483174932957	-1.73829436734654	-1.59735783938977
H	7.75464638879000	-0.93844340051619	-0.98396827282538
C	1.74869187991611	6.28533669297192	-2.79575727092863
H	2.63387251644871	5.63979377123149	-2.90649865716876
H	0.98820308806235	5.93691558667562	-3.51218558099945
H	2.04505921823988	7.30705903133254	-3.08422344743124
C	2.30005538547534	6.76887038900993	-0.37466135160884
H	1.94000784538702	6.77137308892836	0.66625635952401
H	3.20140723071409	6.13773556583065	-0.41603169383638
H	2.60337413407765	7.79682795560992	-0.63192425499973
C	0.01140567702712	7.25697007617969	-1.27227142158854
H	-0.79774873045797	6.98076211464726	-1.96704654621960
H	-0.41110615459666	7.31830032807505	-0.25659273320957
H	0.34755060988619	8.26869912956233	-1.54808054264051
C	-0.90722348730093	-2.34152433496148	1.80382343379753
H	-1.92109958077136	-2.10460881984998	1.44365189768880
H	-0.30747087102689	-2.53984410050117	0.89816971590410
H	-0.95539868367601	-3.27974277629868	2.37860755822987



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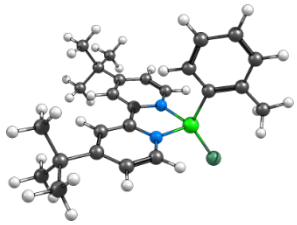
Aryl Chloride RKS 2.0 Å Ni–C distance

Ni	0.00000469694548	-0.00009997227649	0.00087217079841
C	-2.37760056884335	1.41727920835087	0.01773232853815
C	-2.77045973186884	-0.87895611815654	-0.03519455150432
C	-3.75164586504257	1.66630688281888	0.01378225958158
C	-4.14802011858258	-0.67684586400380	-0.04210753505676
H	-2.34435367830657	-1.88198883543815	-0.04947991261306
C	-4.68957198592140	0.62078025041478	-0.01681548112567
H	-4.09301128117879	2.70361935192857	0.03466341987198
H	-4.78822158910819	-1.55986265289561	-0.06704145623046
C	-1.34240882756277	2.45699801839454	0.04701564162629
C	-1.57503680927772	3.83543448094200	0.07832831773572
C	-0.50670812082467	4.74901521768178	0.10567464750656
H	-2.60435587144616	4.20038056378347	0.08155604705070
C	0.95781436255680	2.80737560068764	0.06748327481835
C	0.78412875630896	4.19071891629386	0.09958917615859
H	1.94666467673261	2.34078361264146	0.06128315280620
H	1.67488947235841	4.82004990089809	0.11936454055136
C	-0.00001632789204	-2.00009972232385	-0.00012979488640
C	-0.02012885614027	-2.72290456895650	-1.21111623172477
C	-0.07031331302220	-2.67921623913860	1.22354825203490
C	-0.13857273033766	-4.12519338483461	-1.15579829520696
C	-0.18457049710683	-4.07863670098201	1.26295875178739
C	-0.22616645059369	-4.80303165833842	0.06697044767034
H	-0.15325907518946	-4.69507203686280	-2.09262289348246
H	-0.23429303812089	-4.59641807121572	2.22678944586630
Cl	2.15946269551495	-0.13562291729621	0.00192944783325
N	-1.86504529162909	0.13398157600531	-0.00589892432436
N	-0.07471894124208	1.94068174232352	0.04114911303554
H	-0.02094998035739	-2.12067177556297	2.16424666079796
H	-0.31272351160995	-5.89403779965295	0.08283715528318
C	-6.19656040501340	0.91566661570710	-0.02089649842996
C	-0.77425963948047	6.26166625030509	0.14047349899052
C	-6.54755462667185	1.76519890358627	-1.26789652145739
H	-6.29508242788228	1.23120312314034	-2.19752338874683
H	-6.01141853024581	2.72706117102001	-1.27785985127522
H	-7.62705868839458	1.98738037171525	-1.28560182594258
C	-6.56595654801316	1.70429102516051	1.26031634598015
H	-6.03002292830702	2.66420073339927	1.32449482961533
H	-6.32707494522342	1.12594033750005	2.16669623410137
H	-7.64562928399987	1.92603917370448	1.27286954984035
C	-7.03709791074747	-0.37564443115816	-0.05822955565903
H	-6.85394849326599	-1.01387905006622	0.82095640074659
H	-6.84010968602928	-0.97115538265904	-0.96400707253740
H	-8.10856956834404	-0.12136389431913	-0.06041944514725
C	-1.58149672993214	6.66566995496951	-1.11841274042813
H	-2.55276758065917	6.14950637082931	-1.17132805376676
H	-1.02622931192040	6.43057173776585	-2.04008983302800
H	-1.78215482823594	7.74941693141233	-1.10935213402922
C	-1.59209900462414	6.60520049152552	1.41045126588311
H	-1.04449582930668	6.32628923262757	2.32445782221568
H	-2.56356618128382	6.08707851673134	1.43050585035732
H	-1.79300543293403	7.68817147777077	1.45148548210153
C	0.53162786905479	7.07979828861942	0.16544411062333
H	1.14938439447017	6.90057763354312	-0.72898438423247
H	1.14142235291085	6.85891434960803	1.05599503288331
H	0.29509696673774	8.15505263010846	0.18953930797021
C	0.11060594781991	-2.01626206115483	-2.54134945277335
H	1.07117311143668	-1.47879321163403	-2.59911321840509
H	-0.68227971354287	-1.26161650169875	-2.68322763964503
H	0.05948744441564	-2.72161115428897	-3.38588191600260



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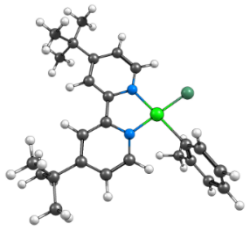
Aryl Chloride Triplet 2.0 Å Ni–C distance

Ni	-0.00034345668129	0.00061355447811	0.00023063429619
C	2.46889925532005	1.22622156571255	-0.63755907947922
C	2.73694470220438	-1.07171742048560	-0.33176538577725
C	3.84185611060566	1.36845734018708	-0.87621244344759
C	4.10628936918074	-0.98709089276282	-0.56810402871228
H	2.25309056655512	-2.02557566408600	-0.10694158705557
C	4.70211696811821	0.25906108680401	-0.85049820151775
H	4.24276325416537	2.36277805232745	-1.08539927449304
H	4.69701519833842	-1.90299554129494	-0.52844575365048
C	1.48574345882195	2.32251586272661	-0.63722751856977
C	1.77601214753516	3.67198839555794	-0.87568236880922
C	0.76649371205768	4.64753896369734	-0.84948566793619
H	2.80788403782996	3.96263545637884	-1.08533242751625
C	-0.76943925545692	2.83821561182004	-0.33059106156386
C	-0.53684126958926	4.19034560346113	-0.56671690018516
H	-1.77010127931126	2.46065437584866	-0.10558147949599
H	-1.38326775018183	4.87689716445868	-0.52670279927419
C	-0.00036773057894	0.00019495810425	2.00023059148485
C	-0.89320151114610	-0.80211789094444	2.75417914189026
C	0.90988101996382	0.81792585575549	2.69057202563583
C	-0.83627355207572	-0.75104856432642	4.16156962575124
C	0.95943715992983	0.86234528740107	4.09198438072261
C	0.07724861643232	0.06970073411054	4.83237214080669
H	-1.52831053495726	-1.37292788670870	4.74219854651241
H	1.68233412227004	1.51180474537954	4.59817439076373
Cl	-1.30486227471549	-1.16970514647242	-1.33871712310754
N	1.92147850125752	0.00037703947582	-0.36818953705231
N	0.20783495526861	1.91124928766682	-0.36754732735489
H	1.61169432667180	1.44854849729526	2.12967032362519
H	0.09742227918919	0.08774696271767	5.92682910533528
C	6.20597516544790	0.43153004467523	-1.11784426432686
C	1.10096314605058	6.12384788627173	-1.11692313917671
C	6.40708467666430	1.03065694865497	-2.53216248026817
H	5.98748692165207	0.37101862353937	-3.30794278961013
H	5.92845177855140	2.01685871570700	-2.63636249566594
H	7.48161635240493	1.16024796411433	-2.74050300858386
C	6.80462295214590	1.39170138022171	-0.05980659972644
H	6.33746789727781	2.38829551529126	-0.09341353907108
H	6.67319546494444	0.99419066594537	0.95887635697578
H	7.88432270998841	1.52576531028102	-0.23619584628374
C	6.96455105745324	-0.90815997182948	-1.04419510101232
H	6.88596778877119	-1.37446200659692	-0.04907432252493
H	6.60370939103466	-1.63015791368050	-1.79414303033638
H	8.03456023338107	-0.73929472584114	-1.24199915836250
C	1.71798590268913	6.25874105782502	-2.53137463346237
H	2.64641622428714	5.67593491365420	-2.63577860780096
H	1.01652331318851	5.91317170545532	-3.30697474499591
H	1.96334376067193	7.31286136153684	-2.73980654474624
C	2.12070458814878	6.61482806014828	-0.05919113791306
H	1.71158098026539	6.52732668602134	0.95961330500214
H	3.06072196835149	6.04231853739409	-0.09306570288031
H	2.37105750448878	7.67361012352097	-0.23567567150538
C	-0.14847439018856	7.02330887196733	-1.04296853626584
H	-0.90557771360754	6.74291668876392	-1.79269600142796
H	-0.62026261814014	6.99585444497601	-0.04770795819183
H	0.13547601411606	8.06865648685857	-1.24091757564795
C	-1.90516122525292	-1.71163646889006	2.09072340378993
H	-2.59495351022885	-1.15280144413252	1.43862975900805
H	-1.42275805800774	-2.45737223132255	1.43918888782730
H	-2.50788307457110	-2.25289203181426	2.83693885835794



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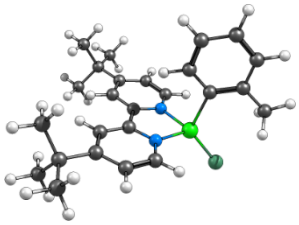
Aryl Chloride RKS 2.2 Å Ni–C distance

Ni	-0.00020430810608	-0.00010885143142	0.00011653007981
C	-2.36772706803534	1.41263124766689	0.01912876933990
C	-2.76111593049140	-0.88493750859964	-0.05032336420421
C	-3.74124272797367	1.66280831310891	0.01126848322988
C	-4.13863867340359	-0.68097197142210	-0.06111314447446
H	-2.33257052172348	-1.88700267695247	-0.06881045425665
C	-4.67909380605197	0.61712553728032	-0.02949708119960
H	-4.08234245904608	2.70018386940789	0.03686830502007
H	-4.77981696338199	-1.56300979200671	-0.09403478024051
C	-1.32807316595997	2.44737451243816	0.05829530537055
C	-1.55144717020819	3.82657274076674	0.09980129930583
C	-0.47741191879499	4.73348817946649	0.13502834403719
H	-2.57879530154462	4.19724922105167	0.10504845122070
C	0.97668893792058	2.78346334705273	0.08360476919629
C	0.81009950567699	4.16724491444783	0.12588822046629
H	1.96245091636072	2.31031921030274	0.07497042275438
H	1.70456379692338	4.79113521140960	0.15120680302216
C	-0.00019858601387	-2.20010881363469	-0.00027780484087
C	0.02368602566605	-2.90062864832187	-1.21841124447639
C	-0.07948882212016	-2.87638944878257	1.21903565338916
C	-0.06462879613247	-4.30644058427257	-1.17578814110347
C	-0.16285434223405	-4.27952627922173	1.24473466932703
C	-0.16099481719940	-4.99323872761875	0.04155925442569
H	-0.04708682973703	-4.87066189833880	-2.11600690510610
H	-0.22145573899502	-4.80728788281421	2.20267101445465
Cl	2.15489840318190	-0.17341036069633	0.00014531984164
N	-1.85696284510281	0.12882801739125	-0.01057747742215
N	-0.06194192691582	1.92357028186996	0.04974257157127
H	-0.06386375823417	-2.32033393583180	2.16200077995777
H	-0.22258842604427	-6.08607815453633	0.04787778485372
C	-6.18601865664888	0.91273463240833	-0.03754544597209
C	-0.73575978129019	6.24738448757765	0.18101755651746
C	-6.53189614657673	1.76963567756176	-1.28094249274186
H	-6.27614682123619	1.24089961606071	-2.21267671976453
H	-5.99530009855900	2.73128590720645	-1.28331649151164
H	-7.61122021420637	1.99243468682339	-1.30145108152572
C	-6.55995039064366	1.69409738462972	1.24680051006596
H	-6.02388274652326	2.65338917420857	1.31860029789622
H	-6.32479846089185	1.11039391985988	2.15072283287042
H	-7.63955846054900	1.91627611502677	1.25651822004426
C	-7.02706421778727	-0.37788180466004	-0.08553463799605
H	-6.84748150695536	-1.02138739107574	0.79054545510732
H	-6.82715802739621	-0.96815942690543	-0.99409544207151
H	-8.09837989116456	-0.12300004685966	-0.09011655416417
C	-1.53911724301471	6.66591051729423	-1.07563013542105
H	-2.51344974377215	6.15607013888060	-1.13349856791976
H	-0.98426159727594	6.43441941157960	-1.99846650956637
H	-1.73324547148998	7.75075522380032	-1.05857298254270
C	-1.55290485019419	6.58647097340481	1.45265014220476
H	-1.00803215181008	6.29740349129348	2.36512877063263
H	-2.52754163828376	6.07415178862869	1.46780196838381
H	-1.74730533673210	7.67030704550074	1.50156543165430
C	0.57509695633606	7.05725927656733	0.21354878106577
H	1.19269343268100	6.88107599456010	-0.68159699423144
H	1.18257136324975	6.82585762167482	1.10301749933517
H	0.34515512614717	8.13373431043382	0.24559141132828
C	0.16546178495899	-2.17294970471088	-2.53509492134431
H	1.11490524036746	-1.61401691696514	-2.56391543448657
H	-0.64074252932657	-1.43314949556858	-2.67875740081148
H	0.14575902330843	-2.86550222641551	-3.39135720457467



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Aryl Chloride Triplet 2.2 Å Ni–C distance

Ni	-0.00168795236911	0.00147877474143	0.00013145350349
C	2.49494127830570	1.23123909595727	-0.46611288519532
C	2.73803566586097	-1.07694924705991	-0.22304323376706
C	3.87750929250232	1.37258650537521	-0.63939500192906
C	4.11719840346384	-0.99280204897540	-0.39280778351405
H	2.24028564021506	-2.03456181353572	-0.05040240285972
C	4.73080333325739	0.25776622866245	-0.61007787957303
H	4.29202425047218	2.37068504945669	-0.79805477818693
H	4.70157534774466	-1.91277387546175	-0.35317013015462
C	1.51781189372609	2.33324064466647	-0.46568368052562
C	1.82359350085115	3.68903675497000	-0.63842627263545
C	0.81898102169825	4.66969570665970	-0.60799148290531
H	2.86409559017251	3.98100396371527	-0.79763587526572
C	-0.74451848771279	2.85078870616602	-0.22119351690247
C	-0.49591596735824	4.21006792363452	-0.39019218659948
H	-1.75475396583176	2.47121562839374	-0.04817049502835
H	-1.33930766309124	4.90030880052190	-0.34957223244601
C	-0.00112220095476	0.00213657754503	2.20013127996893
C	-0.89090629288884	-0.79447380455247	2.95103781187666
C	0.91779654937010	0.82475202005497	2.86043123069020
C	-0.82311423491192	-0.73329786863918	4.35834946791964
C	0.97716431498702	0.87826875583359	4.26298576375457
C	0.09836028572337	0.09189183594528	5.01398924427996
H	-1.51114442692586	-1.34916974604554	4.95025085590437
H	1.70453577514805	1.52948937565452	4.76065469065897
Cl	-1.37084111733222	-1.21391037454054	-1.19356072275829
N	1.92898552066891	0.00051107494337	-0.26297293736519
N	0.22825834189649	1.91854005559606	-0.26227582578802
H	1.61440740821495	1.44806490966966	2.28525807946997
H	0.12725642968584	0.11812044672931	6.10812117043808
C	6.24590987024988	0.42961607284328	-0.80392830109858
C	1.17075745381967	6.15347449814441	-0.80134761307700
C	6.51351901775196	1.07133634457926	-2.18826072952574
H	6.12732401764716	0.43826751760637	-3.00260139831901
H	6.04379213052935	2.06274619625509	-2.28317301259105
H	7.59689759036659	1.20180458193798	-2.34347144096902
C	6.80044186147002	1.35287381193022	0.30957375916273
H	6.34000125965751	2.35287855814674	0.28603148699012
H	6.62096646254770	0.92481810985568	1.30832780362692
H	7.88765662991181	1.48570814114367	0.18642525765940
C	6.99432956553235	-0.91616460152955	-0.73818106729149
H	6.86890148314642	-1.41253308310407	0.23739206954676
H	6.66422172487590	-1.61246331606148	-1.52566870148469
H	8.07291165488142	-0.74766489642556	-0.88249098527603
C	1.83884248421010	6.34294219064965	-2.18602404389163
H	2.76689940027003	5.75804496185942	-2.28178128236494
H	1.16355202498415	6.03549619807940	-2.99998643718103
H	2.09783677592056	7.40299183505412	-2.34107718887731
C	2.15452357178347	6.59303295190917	0.31165443178314
H	1.70888568775140	6.46535948668777	1.31068277891435
H	3.09234700770605	6.01647872574201	0.28698927463783
H	2.41617475054597	7.65667390537057	0.18895777813243
C	-0.07569304804324	7.05758058966448	-0.73422528806294
H	-0.80719881352772	6.81359659205673	-1.52119637182112
H	-0.58265945525858	6.99218922943577	0.24176927786530
H	0.22066580090798	8.10827264932158	-0.87839143640168
C	-1.90457898485349	-1.70292706969298	2.29114026061002
H	-2.59139966395365	-1.14129733262553	1.63844292250098
H	-1.42093763731604	-2.44825640411581	1.64013637934471
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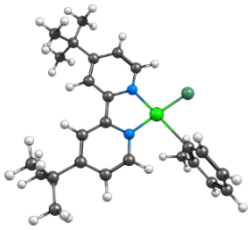

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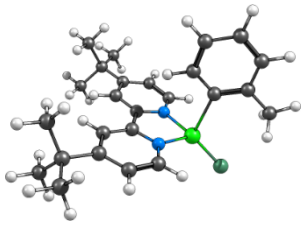
Aryl Chloride RKS 2.4 Å Ni–C distance

Ni	-0.00009344637744	-0.00001549369818	-0.00062395488460
C	-2.36523535235569	1.40251409358776	0.01921321855469
C	-2.75178095078939	-0.89756081985090	-0.06621698969251
C	-3.73916839247594	1.64920447172649	0.00693148646056
C	-4.12986701681762	-0.69641081721943	-0.08161921108961
H	-2.31739680060980	-1.89717427450826	-0.08835434959737
C	-4.67341759840319	0.60039556548713	-0.04437644852338
H	-4.08365012633806	2.68538718583475	0.03704117720456
H	-4.76909042454337	-1.57951081982065	-0.12258782505535
C	-1.32530070916455	2.43676691508216	0.06889452853653
C	-1.54654226578502	3.81560758102072	0.12120476613187
C	-0.47143068990345	4.72112938930102	0.16524312934315
H	-2.57366773608930	4.18704720289218	0.12840439069675
C	0.98176602996038	2.77020827676579	0.09993644100097
C	0.81559794741930	4.15357287524885	0.15304887384201
H	1.96682417081038	2.29560760545681	0.08888430837985
H	1.71060574387759	4.77643308598882	0.18451755431201
C	-0.00001335664635	-2.40001543592967	-0.00010695345305
C	0.08002914720689	-3.07478813888479	-1.22590654443555
C	-0.10206270469905	-3.08034544922630	1.21109807313674
C	0.02089859740762	-4.48332545331324	-1.20084828463160
C	-0.15557320181468	-4.48635625172908	1.21779596137902
C	-0.09823678060109	-5.18421116133575	0.00669444199970
H	0.08016416121932	-5.03731049088852	-2.14550603221887
H	-0.23356685563548	-5.02716525633020	2.16710646638534
Cl	2.15188210200149	-0.19706988246690	-0.00143360257312
N	-1.85236149771034	0.12009336406372	-0.01617520282291
N	-0.05846609206666	1.91206981115892	0.05781262634531
H	-0.13008160508690	-2.53202364230502	2.15803705622428
H	-0.13574417194687	-6.27814257131324	-0.00056621366601
C	-6.18121396826898	0.89185875352877	-0.05732304754248
C	-0.72823987605919	6.23483013056674	0.22354272494055
C	-6.52398663111751	1.75521548517368	-1.29711569657414
H	-6.26262587665493	1.23278717514391	-2.23084670364894
H	-5.99017008430527	2.71839211871372	-1.29138176573505
H	-7.60383481746910	1.97507346249947	-1.32107688721923
C	-6.56295635583676	1.66447245375376	1.23001977710063
H	-6.02994321020682	2.62481958163152	1.30993105522539
H	-6.33016254042300	1.07601909610390	2.13146954308472
H	-7.64320939665312	1.88358096961114	1.23629304994534
C	-7.01849306988093	-0.40071726874575	-0.11675094586238
H	-6.84108710773840	-1.04898612064609	0.75625612152141
H	-6.81303690686654	-0.98500144858320	-1.02794361948807
H	-8.09045549561761	-0.14867748248548	-0.12454692439427
C	-1.52943162452614	6.66479423469053	-1.03063675789924
H	-2.50421575325364	6.15647635530163	-1.09412818243794
H	-0.97354481844433	6.44050311812419	-1.95462853035798
H	-1.72250294103865	7.74965216035646	-1.00471654198858
C	-1.54676314047577	6.56423065562448	1.49685096796487
H	-1.00345894359360	6.26697261511327	2.40762875078055
H	-2.52198306290810	6.05288031638795	1.50640841866070
H	-1.74008869346372	7.64782830934104	1.55453563644176
C	0.58344308734705	7.04297633314028	0.26464980448522
H	1.20207158688560	6.87369458484992	-0.63111863179838
H	1.18945532730014	6.80345630035785	1.15296919951378
H	0.35461068120466	8.11938885873300	0.30544212987444
C	0.24693253513691	-2.32271807746427	-2.52509085654292
H	1.18475693172488	-1.74410274833806	-2.51369179633275
H	-0.56983977823738	-1.59668586546177	-2.67787111181921
H	0.26674457339750	-2.99977276381763	-3.39359561718724



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Aryl Chloride Triplet 2.4 Å Ni–C distance

Ni	-0.00033327531133	0.00039997778303	0.00015358543248
C	2.51298623249766	1.23475554280655	-0.28942092930195
C	2.73911109843192	-1.08089016748188	-0.11135022660404
C	3.90183324670844	1.37642055795075	-0.39716494189791
C	4.12491175732003	-0.99622445123151	-0.21373147368527
H	2.23195107237742	-2.04178100843601	0.00748877720270
C	4.75066208066023	0.25801347028665	-0.36462560806308
H	4.32508776147151	2.37764397191361	-0.50525822031622
H	4.70484962506387	-1.91902794342803	-0.17464635049458
C	1.53873061716178	2.33964854844818	-0.28871407751395
C	1.85309561295889	3.69991670740185	-0.39557353906163
C	0.84975521577871	4.68206654083057	-0.36188501418659
H	2.89939177101789	3.99454067557019	-0.50402670145422
C	-0.73026167128453	2.85374779554067	-0.10891039953792
C	-0.47285353075479	4.21810886319793	-0.21054246183176
H	-1.74702338054009	2.47080827184313	0.01024956226360
H	-1.31579952165603	4.90893613505728	-0.17057534976598
C	-0.00025403681827	0.00018076398129	2.40015357336634
C	-0.89586321861402	-0.78714161108814	3.14431360014892
C	0.93102223077594	0.81902702760450	3.03715235170505
C	-0.81994070547722	-0.72028286446491	4.55180529877515
C	0.99642996343343	0.87659264325664	4.44084654638347
C	0.11337972104715	0.10028073140735	5.19757745545184
H	-1.51017125650359	-1.32706007034276	5.15070585763721
H	1.73150668742226	1.52290483955783	4.93376093519236
Cl	-1.42137747155335	-1.25407191000864	-1.05499658488674
N	1.93426951067222	0.00016752105011	-0.15376760784819
N	0.24149186509379	1.91991800438949	-0.15259768147222
H	1.62817019484840	1.43205742845967	2.45176079219433
H	0.14808684070830	0.13086177846902	6.29140849463794
C	6.27328893097152	0.43012341451986	-0.48510239972805
C	1.21096902983854	6.17127703310790	-0.48177611886351
C	6.60414642385705	1.11021109422782	-1.83703085079084
H	6.25426470288997	0.50155109087432	-2.68569717179397
H	6.14046340434353	2.10514387879810	-1.92464515224266
H	7.69360788731015	1.24218971508391	-1.93949882206220
C	6.77934785267810	1.31932023698419	0.67810899204974
H	6.32367555969867	2.32164746545358	0.66184857379809
H	6.55318154309279	0.86423953163399	1.65517846320830
H	7.87145093369912	1.45080515030379	0.60830015233474
C	7.01508959534309	-0.91953997373502	-0.42434713637258
H	6.84459086895599	-1.44305625245078	0.52996193679322
H	6.71943262213670	-1.59195590378601	-1.24556446146617
H	8.09945570110735	-0.75070833895378	-0.51495721687240
C	1.92670321601323	6.41506980476315	-1.83377172650491
H	2.85579538964635	5.83058645913980	-1.92190119142047
H	1.27882326031925	6.14447766131448	-2.68238831358838
H	2.19391894419768	7.47950469662318	-1.93582458784312
C	2.15679216433792	6.56166961794242	0.68133946709460
H	1.67735056921534	6.39359773361188	1.65847609765649
H	3.09433604262082	5.98440162571119	0.66445801921644
H	2.42363916751397	7.62883216125500	0.61201458552797
C	-0.03527197236564	7.07606957672035	-0.42024009550982
H	-0.73966122886591	6.86725750948811	-1.24133416399927
H	-0.57570733609042	6.97199067968520	0.53418818028546
H	0.26786598377133	8.13083702414552	-0.51046295757589
C	-1.91739170637064	-1.68539627505681	2.48408695137284
H	-2.59649689269058	-1.11463978422370	1.83131861545725
H	-1.43808810846514	-2.43283187061550	1.83244112853718
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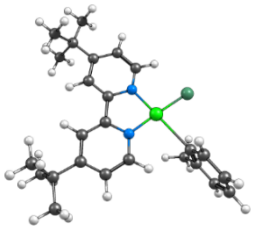

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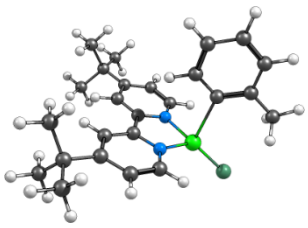
Aryl Chloride RKS 2.6 Å Ni–C distance

Ni	-0.00770113267897	0.05520537153822	-0.01332244578519
C	-2.37408388205711	1.44577168565359	0.01867323929238
C	-2.75152155587921	-0.85760293743260	-0.06284724153208
C	-3.74888112781657	1.68699357481028	0.01066752798148
C	-4.13047785617331	-0.66137251169919	-0.07341711681328
H	-2.31044268079458	-1.85440087771482	-0.08494175360262
C	-4.67861067914255	0.63364755906665	-0.03619900581071
H	-4.09799626414217	2.72166614075435	0.04014152322200
H	-4.76676204322600	-1.54673296767020	-0.11075389370268
C	-1.33578053518646	2.48232714724680	0.06396139127244
C	-1.55817692447162	3.86055427532408	0.12097972634267
C	-0.48405758274071	4.76769007016597	0.15984270729777
H	-2.58584298090329	4.23036528281285	0.13649583223060
C	0.97259085859237	2.81942968951109	0.08013889961759
C	0.80389003532536	4.20229195945503	0.13740523166729
H	1.95812660789498	2.34615677840156	0.06124627751129
H	1.69798967315434	4.82669472791733	0.16418628828236
C	-0.01350179958355	-2.54474636933309	0.00141873360247
C	0.12534281543865	-3.19652318582801	-1.22814364331755
C	-0.14838576636645	-3.23005376124726	1.20326135295173
C	0.09043589213079	-4.60673275858388	-1.21816728657769
C	-0.17692790294485	-4.63787939868382	1.19369832142954
C	-0.06059799463259	-5.32088391456953	-0.02166806832368
H	0.19407738132103	-5.15074951381670	-2.16488422345331
H	-0.28136335002364	-5.19011110601179	2.13394141829666
Cl	2.14104300786878	-0.15797667056645	-0.03446514919045
N	-1.85744875868983	0.16530457348772	-0.01733674957037
N	-0.06727829187728	1.96019316402783	0.04312008324825
H	-0.22282461810872	-2.68992912505833	2.15234786719487
H	-0.07803982237588	-6.41515492353291	-0.04072788991135
C	-6.18766350520227	0.91897052184738	-0.04496225739874
C	-0.74295057052942	6.28082887165169	0.22332607132301
C	-6.53765534575781	1.77875028828682	-1.28524394260893
H	-6.27711353362370	1.25567815118882	-2.21884088980161
H	-6.00768997733906	2.74406662231751	-1.28292632343880
H	-7.61843888061369	1.99423691956728	-1.30625469264435
C	-6.56858267329469	1.69227072236625	1.24221986222929
H	-6.03918483740374	2.65487309247626	1.31894930480655
H	-6.33077456138849	1.10626620057900	2.14395829171958
H	-7.64966441527536	1.90710301447855	1.25137980660119
C	-7.01990936671654	-0.37703959692990	-0.09962642739690
H	-6.83726531912161	-1.02317129176171	0.77388376722213
H	-6.81501529323450	-0.96200129309947	-1.01050628998303
H	-8.09287722490138	-0.12926283297725	-0.10449078878676
C	-1.55144968640571	6.71244632016281	-1.02560539133149
H	-2.52563937202808	6.20249622898690	-1.08522924542389
H	-1.00001659847373	6.49139321013089	-1.95303885362221
H	-1.74633950563419	7.79688645435535	-0.99602675690213
C	-1.55526108016201	6.60608799332866	1.50167325122200
H	-1.00662150744918	6.30788236871713	2.40893466086837
H	-2.52957867862152	6.09311633070000	1.51539030565746
H	-1.75013028133336	7.68922259996473	1.56263507011024
C	0.56767600296570	7.09092107860792	0.25949330836034
H	1.18152632594028	6.92538495933251	-0.64025329981659
H	1.17898761436288	6.84958812910293	1.14368335807399
H	0.33741739418089	8.16684078614695	0.30483281745249
C	0.32616497193676	-2.42371772934538	-2.50987587062500
H	1.25219740539922	-1.82908188277525	-2.45500623600764
H	-0.49738622414490	-1.70934595880642	-2.67932060038218
H	0.38823675595829	-3.08727949902580	-3.38672751332689



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Aryl Chloride Triplet 2.6 Å Ni–C distance

Ni	-0.00021978645376	-0.00013033518081	0.00011320739657
C	2.51823574713735	1.23638711028594	-0.12920595490962
C	2.73490987208914	-1.08343180623143	-0.00913317878795
C	3.90958579165888	1.37854600180062	-0.18319740895554
C	4.12389625585594	-0.99838685522527	-0.05572339426561
H	2.22291723685736	-2.04641287613001	0.06306159591772
C	4.75608888220771	0.25782761382240	-0.14979017111257
H	4.33725180131381	2.38163694637861	-0.24868133018702
H	4.70108275217847	-1.92301739323863	-0.01848225164109
C	1.54425181613395	2.34219248196074	-0.12807807340990
C	1.86096945422215	3.70450517605551	-0.18043590507986
C	0.85618870363724	4.68575764439253	-0.14479373472989
H	2.91001123904900	4.00210588904217	-0.24628022743098
C	-0.72947958118301	2.84995853138691	-0.00536976599915
C	-0.46972905373462	4.21712905248171	-0.05035035515398
H	-1.74936682973862	2.46364682380802	0.06721559548772
H	-1.31403772496335	4.90639431305856	-0.01150013547548
C	-0.00006969583450	0.00053349796149	2.60011311927436
C	-0.90118927285451	-0.78117714346536	3.33596191985533
C	0.93995388202431	0.81683943097047	3.21889106766440
C	-0.82037018353918	-0.71052423141149	4.74369795257889
C	1.00790156836028	0.87629664821230	4.62366644256914
C	0.12097178764858	0.10667911331203	5.38309809468972
H	-1.51253445468887	-1.31099685782230	5.34688051458450
H	1.74790646194919	1.51879845635186	5.11429429385382
Cl	-1.45876529497842	-1.28723611055073	-0.93297054964088
N	1.93235800434565	-0.00019168922588	-0.05097105308431
N	0.24366170120542	1.91704305944117	-0.04921898990084
H	1.63738368562077	1.42222818310176	2.62611027707778
H	0.15895334254857	0.14000558779376	6.47669235054713
C	6.28216722933276	0.43039536948624	-0.20954362638695
C	1.22006645230855	6.17792249763495	-0.20251701089325
C	6.66308561135284	1.14492817708275	-1.53017708556814
H	6.34479198394415	0.55884918401675	-2.40673277815957
H	6.20308316047491	2.14230457196743	-1.60904379115923
H	7.75562141596203	1.27831152107399	-1.58879845061222
C	6.74582493909238	1.28811479411453	0.99427192967742
H	6.29199461777912	2.29138977488826	0.98738665096826
H	6.48334358180106	0.80819697000753	1.95013489128328
H	7.83987754691698	1.41934731579603	0.96816042979478
C	7.02014928991728	-0.92167605423216	-0.15674158242606
H	6.81403988812187	-1.46956788125440	0.77662215019319
H	6.75443032075847	-1.57193821654063	-1.00557834553606
H	8.10727238100626	-0.75251918438360	-0.20283258866694
C	1.97587268013987	6.46767165292189	-1.52329235231452
H	2.90712706675184	5.88552391652884	-1.60385752904486
H	1.35357278400528	6.22735639216959	-2.39972891757133
H	2.24609898298580	7.53471206564650	-1.58041766454183
C	2.13045572947412	6.52770109995815	1.00110790680508
H	1.62209340170159	6.32631315731808	1.95708576744189
H	3.06842287000830	5.95094145542011	0.99247905486844
H	2.39867445304583	7.59648989786849	0.97649122298517
C	-0.02793907111189	7.08065838337821	-0.14720731894416
H	-0.70727659054978	6.90062653123694	-0.99577519736936
H	-0.59669271283064	6.94384755641031	0.78640365459917
H	0.27711149055904	8.13779317804370	-0.19179225040363
C	-1.92691102561183	-1.67154523478599	2.67227309901711
H	-2.59914800504043	-1.09366115358423	2.01873048206684
H	-1.44921033126913	-2.41967719502439	2.02034762018582
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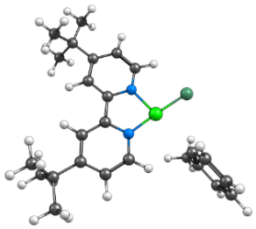

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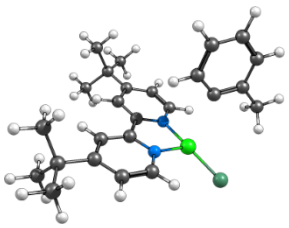
Aryl Chloride RKS 2.8 Å Ni–C distance

Ni	-0.00662734502564	0.11132445583695	-0.02164034320079
C	-2.37716470609225	1.48780067184539	0.01989688135138
C	-2.74367040469652	-0.81890972466228	-0.05908141405939
C	-3.75306999482194	1.72227657275186	0.01714062983605
C	-4.12366469022095	-0.62881277079481	-0.06387349526522
H	-2.29535883534303	-1.81256944241498	-0.08265529964038
C	-4.67741439267983	0.66379868171177	-0.02518308553332
H	-4.10756792339623	2.75512305426750	0.04705558375926
H	-4.75613564840590	-1.51701285679449	-0.09792293094947
C	-1.34187015104974	2.52792949511777	0.06052890848842
C	-1.56789458281861	3.90531788920580	0.11913665982728
C	-0.49651510610371	4.81602176887497	0.15276160353812
H	-2.59673029525863	4.27170454092560	0.13997160358852
C	0.96672945905118	2.87263178108812	0.06542079055782
C	0.79317424662068	4.25481243526661	0.12371835599513
H	1.95369905849542	2.40287271575307	0.04145924548312
H	1.68534161376475	4.88218023398611	0.14604021425896
C	-0.03196248019987	-2.68844330588573	0.00402279354473
C	0.16994855629585	-3.31284041278286	-1.22843116467314
C	-0.21556834708677	-3.38559643960807	1.18987224373156
C	0.14891555235054	-4.72396277651691	-1.24001280856243
C	-0.22948381810327	-4.79433395815434	1.15761291236340
C	-0.04954266683539	-5.45647397750543	-0.06144781447288
H	0.30072389471441	-5.25330287552085	-2.18666613373905
H	-0.37243725768299	-5.36198725763682	2.08361197696356
Cl	2.13906233665843	-0.11315685771548	-0.05562145140140
N	-1.85564670816258	0.20979933151539	-0.01748597789382
N	-0.07108218941207	2.01010807930963	0.03343876541079
H	-0.33989866528819	-2.85932264570560	2.14160304797533
H	-0.05475075027190	-6.55045240457381	-0.09723906932078
C	-6.18793520587527	0.94177532152420	-0.02790221652151
C	-6.76003092790165	6.32825771687603	0.21794957438480
C	-6.54721932003899	1.79854217860386	-1.26762285733339
H	-6.28803484458107	1.27574547340862	-2.20174925903286
H	-6.02199172472358	2.76645211015646	-1.26852424293796
H	-7.62911497187082	2.00870941311453	-1.28434074027432
C	-6.56722835258551	1.71455987994140	1.26007444121220
H	-6.04229767683552	2.67985441438936	1.33362452233451
H	-6.32282553305745	1.13067033805268	2.16142140204107
H	-7.64929776581123	1.92407794823403	1.27349956065109
C	-7.01411229862674	-0.35830037154137	-0.07776187541646
H	-6.82472427784123	-1.00264546934062	0.79563099859355
H	-6.81026285447130	-0.94321526340725	-0.98889943373674
H	-8.08826414524424	-0.11569264728286	-0.07836373540022
C	-1.57660965405824	6.75750300835187	-1.02654731574529
H	-2.54945269084186	6.24441083142110	-1.08110043179668
H	-1.02942630653516	6.53849502744119	-1.95697747482132
H	-1.77489295527400	7.84128511523708	-0.99564194680676
C	-1.56656537344786	6.65057921031726	1.50069445096260
H	-1.01208368374597	6.35408466552958	2.40495644981849
H	-2.53909076905768	6.13436586019694	1.51954295746884
H	-1.76474315781600	7.73304095674088	1.56287594825920
C	0.54811910514692	7.14262369158485	0.24726855181979
H	1.15773767692521	6.97918972977082	-0.65573667704407
H	1.16487556107943	6.90327452750745	1.12821209986721
H	0.31457839954887	8.21777355457894	0.29391554048715
C	0.41988484167948	-2.51509829414769	-2.48587578676405
H	1.33452741751129	-1.91050975193542	-2.37731728342880
H	-0.40413898191943	-1.80701083127365	-2.67735557361207
H	0.52887346527438	-3.16146958723449	-3.37090442518940



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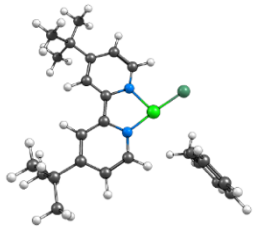
Aryl Chloride Triplet 2.8 Å Ni–C distance

Ni	-0.23339825295833	0.31672933413110	0.02980916851563
C	2.34793557386758	1.38957362758977	-0.09583732301939
C	2.42424387060095	-0.93439012361820	0.06179349076132
C	3.74503372113968	1.45004798822525	-0.10245612400073
C	3.81596179813310	-0.93149091168077	0.05231954754645
H	1.85987884442203	-1.86707862359288	0.13718227341958
C	4.52506731188869	0.28341027110357	-0.03096719540341
H	4.23084025699005	2.42714453814728	-0.15574617419137
H	4.33550230506425	-1.88844322717410	0.11549319775323
C	1.44538690485343	2.55344175159496	-0.14935461660494
C	1.83908493205219	3.88800155500941	-0.29346756178928
C	0.89017525894823	4.92564028049674	-0.31116270873763
H	2.90168106092656	4.11991908605922	-0.39607458408230
C	-0.79780318563861	3.19580748263337	-0.05521655756640
C	-0.45916062491546	4.54165313324498	-0.18249277207213
H	-1.83637165085610	2.86610721394867	0.03206373428872
H	-1.26188803966610	5.28002092217764	-0.18349897280011
C	0.04760428065433	-0.07846333729126	2.78750028860161
C	-0.42382478066778	-1.26930111876788	3.34609644579490
C	0.63131896437956	0.93104609645760	3.53899297293963
C	-0.28599642143763	-1.41652809284375	4.74348638621671
C	0.76008487449486	0.76590208840265	4.93213122975155
C	0.29763604862006	-0.41238146159567	5.52795667634298
H	-0.64746228612970	-2.33549764904838	5.22149616479036
H	1.21368050893473	1.55587722075782	5.54131009839728
Cl	-2.18857756167897	-0.35858598522227	-0.56761921247504
N	1.68190292379901	0.19163034740721	-0.01452687583871
N	0.12392978849624	2.21226250013450	-0.03696196221555
H	0.98824210595053	1.85421198174102	3.06763142813237
H	0.38760786613582	-0.55262127128879	6.60984144105327
C	6.05941503629879	0.36687991339691	-0.03366836796526
C	1.33804834081130	6.38762214694195	-0.46775122222377
C	6.53239532143830	1.05824674348665	-1.33662796129554
H	6.21495297260998	0.49193895004074	-2.22645276714439
H	6.13474674655880	2.08079094994817	-1.43070478846275
H	7.63228589877557	1.12813115323845	-1.35258911516402
C	6.52558017251570	1.19581481172988	1.18932959354743
H	6.13025903045328	2.22336976873197	1.16756406285401
H	6.19878511590850	0.73160181718546	2.13297343000830
H	7.62563659709786	1.26390175082054	1.20559900306094
C	6.71447584495446	-1.02608445665272	0.04380079900886
H	6.44418888928144	-1.55964657129071	0.96902298037446
H	6.44034168701986	-1.66065678929927	-0.81428466750291
H	7.81065131919757	-0.92137416493127	0.03576722176743
C	2.08987596298790	6.54879785833289	-1.81263174065213
H	2.98577033649399	5.91079547174436	-1.86566759355670
H	1.44233348506970	6.28890355006062	-2.66481664646048
H	2.41847867504968	7.59297746040705	-1.94124719282084
C	2.28472851375597	6.75901624697380	0.70086397823886
H	1.77892533367128	6.65112393433120	1.67327134093915
H	3.18666199160863	6.12766194706388	0.72023653107678
H	2.61532775291211	7.80595098561244	0.60386069564891
C	0.14506385233706	7.36337187440315	-0.45668172721497
H	-0.55455338240889	7.17171820597873	-1.28592680151705
H	-0.41863322663411	7.31750967075040	0.48883600170297
H	0.51011292297228	8.39612410596760	-0.56956735111391
C	-1.05033661993656	-2.35884311282704	2.50515181775003
H	-1.85016324184354	-1.95960534446841	1.86315586867779
H	-0.30842314750713	-2.81828977234936	1.82854855475449
H	-1.47045543285360	-3.16347238946739	3.12874259017545



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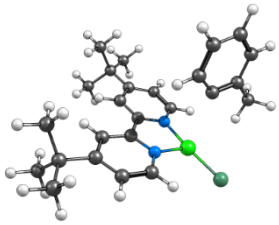
Aryl Chloride RKS 3.0 Å Ni–C distance

Ni	-0.00053890017017	-0.00035490097041	0.00237186298748
C	-2.40522862362958	1.31198629538896	0.02280342063902
C	-2.71026434576332	-1.00270530322071	-0.10464061394748
C	-3.78639495496829	1.51121712871430	-0.00132483471142
C	-4.09440422651761	-0.84746865395024	-0.13172140400797
H	-2.23372761578673	-1.98311193725512	-0.13766012829969
C	-4.68172104218000	0.42986139889393	-0.07961755174112
H	-4.16838305358899	2.53381332120895	0.04039545058057
H	-4.70322192617393	-1.75052151554081	-0.19389994457738
C	-1.39661029567407	2.37646944360363	0.10003973432094
C	-1.65690777487789	3.74675160944162	0.17872280352854
C	-0.60900147029658	4.68274124428418	0.24556764565992
H	-2.69475133779749	4.08737161076728	0.18914629131831
C	0.90346219498387	2.77735526180657	0.14918094666719
C	0.69448458423809	4.15360011364232	0.22810823307923
H	1.90209717297316	2.33294093122101	0.13371471771587
H	1.57046530149370	4.80204684077325	0.27562908875712
C	-0.00082103157137	-3.00035319511116	-0.00081609105138
C	0.31299130344723	-3.57801282400207	-1.23079459712940
C	-0.26240714201741	-3.73022252847092	1.14800944234412
C	0.32691025277117	-4.98887954215049	-1.28219032509111
C	-0.24011442095790	-5.13824815107652	1.07543954124860
C	0.05276324661763	-5.75917614020731	-0.14332727354466
H	0.56576832135518	-5.48743157102742	-2.22972744089504
H	-0.44375135007132	-5.73628124206229	1.97058085102263
Cl	2.14639426363309	-0.19191946529427	0.00378859330478
N	-1.85107895429131	0.04854650628006	-0.02707868157313
N	-0.11259433403914	1.89046933311961	0.08512549916017
H	-0.47477403464797	-3.23471856573486	2.10098455831561
H	0.07670057447400	-6.85148365603410	-0.20955869649859
C	-6.19870598706274	0.66896323499938	-0.10469846675324
C	-6.91065283396444	6.18669412238427	0.33223852743265
C	-6.55832504425926	1.53835843115253	-1.33549021977534
H	-6.26926189577064	1.03931755931477	-2.27382688091559
H	-6.05864428124712	2.51937482175740	-1.30995171862974
H	-7.64486484575427	1.72084441790127	-1.36799924564888
C	-6.62033704307250	1.40856521947864	1.18962703615537
H	-6.12240344655664	2.38573521150527	1.28914811884310
H	-6.37622808812443	0.81531067854835	2.08491304962950
H	-7.70760945341490	1.58957744050553	1.18752646645450
C	-6.98988589886349	-0.65073574833100	-0.19201749721242
H	-6.79919989049215	-1.30552758968895	0.67328085413772
H	-6.75517639802079	-1.21393660027753	-1.10938692338166
H	-8.06977780540152	-0.43570170297157	-0.20761586648569
C	-1.71771035346242	6.61763798514689	-0.91787916761914
H	-2.67656979922485	6.08193047822700	-0.99713395094729
H	-1.15053891304122	6.42855887971502	-1.84288625402795
H	-1.94326687137880	7.69551239609460	-0.87154882211976
C	-1.74518593784334	6.46682796124111	1.60699609489976
H	-1.19818974212810	6.16783931135497	2.51498313855186
H	-2.70504557797452	5.92717268519246	1.60093408015451
H	-1.97061573720272	7.54293498506086	1.68459222542197
C	0.37642111595759	7.03199848796451	0.39684358615043
H	1.00420287734715	6.89934171467312	-0.49874447035370
H	0.98476425541530	6.79242290338457	1.28355665974771
H	0.11572524634562	8.10014499513538	0.45803975737642
C	0.64069896010306	-2.73582536862322	-2.44067734021337
H	1.52578156606985	-2.11097716567511	-2.24121720854679
H	-0.18530087674957	-2.04332470963478	-2.67530633769738
H	0.83684905780583	-3.35164145157270	-3.33240983420929



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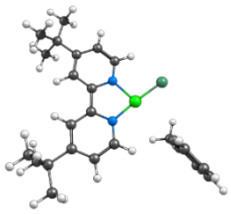
Aryl Chloride Triplet 3.0 Å Ni–C distance

Ni	-0.30654256249307	0.32426947963475	-0.11818174730212
C	2.28667169066254	1.36524398706220	-0.13404719117021
C	2.32940525954338	-0.96125167165738	-0.01057726826229
C	3.68333163912174	1.40723950257852	-0.11745601628568
C	3.72145016959098	-0.97621862354421	0.00758054611847
H	1.75277842377944	-1.88843051201726	0.03535060739238
C	4.44766859694098	0.22945510435530	-0.04516181526184
H	4.18273763847227	2.37816273594398	-0.15635293077841
H	4.22698670013327	-1.94101235695309	0.06591376055834
C	1.40016974251561	2.54104462627337	-0.19755577169338
C	1.81343128893477	3.87347373598046	-0.29185412987574
C	0.87689581920707	4.92222141219178	-0.33366494523330
H	2.88214023304717	4.09610417338970	-0.33398185457278
C	-0.83796451094528	3.20530400201571	-0.19761176279466
C	-0.48052882783387	4.54993667244389	-0.28043520582903
H	-1.88305439991227	2.88603453710729	-0.16623926065746
H	-1.27522293591495	5.29660534623470	-0.30573587103980
C	0.03062905889372	0.09715109722025	2.85414604964437
C	-0.17221416120251	-1.19067440283602	3.34361438672952
C	0.37476111576979	1.18051919492321	3.64928871627441
C	-0.00316873807393	-1.37254943837142	4.73551096326342
C	0.53704476873734	0.97813455131130	5.03254889755344
C	0.34678777226051	-0.30297742621667	5.56794750855571
H	-0.15421385924252	-2.36978792832579	5.16790099736049
H	0.80626136061880	1.81693840834198	5.68416758457215
Cl	-2.23314334616231	-0.43187442822788	-0.68302338996356
N	1.60205385149242	0.17568616714522	-0.07703735511230
N	0.07164096349418	2.21067255291052	-0.15510974210886
H	0.51763403214027	2.17939696375645	3.22200597273730
H	0.46859349141769	-0.46960533169278	6.64287501884717
C	5.98260165122551	0.29338671839914	-0.01948966357185
C	1.34659090027479	6.38215584940634	-0.43518659973128
C	6.48793472667830	0.99078197533108	-1.30702779350207
H	6.17960009419101	0.43688861351883	-2.20780567032666
H	6.10495712128162	2.01914805541973	-1.39854154168016
H	7.58874831648346	1.04683525326138	-1.30245960294471
C	6.43702359106152	1.10484482205348	1.21954295175447
H	6.05464510116076	2.13733398951406	1.20074729026896
H	6.08758610177931	0.63598879420134	2.15271015707740
H	7.53737783257526	1.15918694407050	1.25602789965948
C	6.61844079837124	-1.10851527275036	0.05645858834276
H	6.32312727875255	-1.64765257544732	0.97075424590454
H	6.35318287187299	-1.73096911223454	-0.81322150255992
H	7.71581459027202	-1.01786091033249	0.07087318132021
C	2.16640572259805	6.56422990910514	-1.73697216646469
H	3.05722690057101	5.91737024438539	-1.75941495233338
H	1.55973371943193	6.33023068672290	-2.62595975206280
H	2.51176796551693	7.60715905086566	-1.82580917224210
C	2.23735998455309	6.71797800932568	0.78693188800558
H	1.68224452309630	6.59575128908355	1.73031663112420
H	3.13030873518515	6.07574301129912	0.83795460175889
H	2.58361664475997	7.76277203424872	0.72910299681520
C	0.16426908518183	7.37048092442306	-0.46194655569608
H	-0.49485328006768	7.20444231280352	-1.32904866155710
H	-0.44648386394491	7.31019479139683	0.45305765480116
H	0.54455404085180	8.40143474258741	-0.53352848276019
C	-0.55909354715347	-2.34305968858741	2.44307201259200
H	-0.64025583066622	-1.99735891785407	1.40262632896746
H	0.17647352515094	-3.16475219008685	2.48969382072122
H	-1.53913243103860	-2.76545915210825	2.71954554625357



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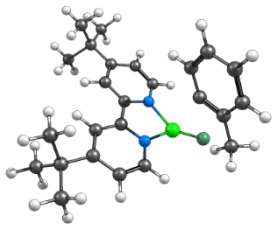
Aryl Chloride RKS 3.2 Å Ni–C distance

Ni	-0.02966723908317	-0.06228859722122	-0.02929559348089
C	-2.48565865207225	1.14725769034812	0.00810447418419
C	-2.69452832086321	-1.17792342760763	-0.14126795509181
C	-3.87387033521965	1.28926593965068	-0.01226800381691
C	-4.08397889030588	-1.07954674365756	-0.16402878810646
H	-2.17564411395884	-2.13651128745845	-0.18483351182174
C	-4.72336746064478	0.17195754035860	-0.09866690496643
H	-4.29824198591277	2.29461679161069	0.03867994925721
H	-4.65512640599281	-2.00632700524857	-0.23379136545683
C	-1.52035540289928	2.25093187934497	0.09280608156559
C	-1.83443719970694	3.60869318832633	0.18796023228499
C	-0.82437926952524	4.58515349857608	0.25937427106214
H	-2.88502646419738	3.90731271125024	0.20818106274333
C	0.76319554738997	2.74345114902550	0.13541059245239
C	0.49928051752826	4.10919251787949	0.22944347177059
H	1.77879842299587	2.34021428062592	0.11116772938142
H	1.34865508014563	4.79196495289949	0.27918263832770
C	0.02831951057755	-3.26176290734091	-0.02796442534279
C	0.40940094590461	-3.78825317354695	-1.26068636776737
C	-0.26103002681338	-4.02949120760986	1.08743309507535
C	0.46661891166919	-5.19637786719951	-1.35296976044041
C	-0.19521531579132	-5.43411078377188	0.97347712177524
C	0.16696084638193	-6.00804854840715	-0.24966139981324
H	0.75914061106677	-5.65927512711533	-2.30367951572965
H	-0.42032658372590	-6.06531450462343	1.84040041155008
Cl	2.11827875986026	-0.19175076191128	-0.03438625785606
N	-1.88045005406950	-0.09162812523153	-0.05455535830305
N	-0.21750727398503	1.81752327840768	0.06695802357247
H	-0.52809852912914	-3.57029028110495	2.04524581168437
H	0.22508541391758	-7.09673648617337	-0.34714873629900
C	-6.24908813332774	0.34797521661191	-0.11906388827290
C	-1.18553538350415	6.07477979176419	0.36410648543590
C	-6.64686032559229	1.21249139434573	-1.34152960310886
H	-6.33925030108239	0.73411784271942	-2.28471720097152
H	-6.18823548038468	2.21313907478716	-1.30813166563374
H	-7.74008924511838	1.35003577988728	-1.37064213326062
C	-6.69858479720175	1.05793339456037	1.18245232015978
H	-6.24207440555913	2.05432057700067	1.28967830782030
H	-6.42788528299548	0.46772410787587	2.07208510417745
H	-7.79250159696247	1.19302559847660	1.18381254368590
C	-6.98486978423861	-1.00268038330196	-0.21674534103716
H	-6.76492502357837	-1.65669713052674	0.64216202458760
H	-6.72930109124780	-1.54741833120304	-1.13966315166892
H	-8.07280085555641	-0.83263299648707	-0.22811902880012
C	-2.01634581971680	6.48645100949049	-0.87692175866761
H	-2.95336452325906	5.91353237298233	-0.95716499624872
H	-1.44729917616728	6.33050671608082	-1.80694455954012
H	-2.28475399860464	7.55379867849368	-0.81740199484094
C	-2.02325750907487	6.30744401272625	1.64630437213123
H	-1.45960620769717	6.02066625135823	2.54801730787402
H	-2.96089031409759	5.73005881289250	1.63932851495273
H	-2.29094950006443	7.37277568696685	1.73702686560357
C	0.06700131381961	6.97031281718461	0.43112809832021
H	0.69448310911501	6.87252623050323	-0.46914550156953
H	0.68945859240392	6.74598419764067	1.31201613122709
H	-0.23592602369177	8.02641785007359	0.50527469506739
C	0.76085661207037	-2.89783595681143	-2.42893050369406
H	1.62258365847055	-2.25948894686277	-2.17706247176900
H	-0.07257890313193	-2.21591063595442	-2.66779752846414
H	1.00238950943481	-3.47787557934932	-3.33342366088961



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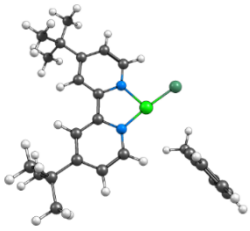
Aryl Chloride Triplet 3.2 Å Ni–C distance

Ni	-0.00005425733343	0.00014639961367	0.00003391203456
C	2.51124187063200	1.22593722527406	0.10896718256125
C	2.71328450437449	-1.07077027010542	-0.25690651268584
C	3.90010330456494	1.37461233815992	0.05412221535019
C	4.10303584578800	-0.97984535343981	-0.31362852935321
H	2.19093021632313	-2.02306230825949	-0.38161862406695
C	4.74057737445095	0.26641019727967	-0.15822676729223
H	4.33285473465289	2.36989317673712	0.17959077972989
H	4.67546232468588	-1.89295968338359	-0.48192775196823
C	1.53453499452331	2.30762052120006	0.32808261939946
C	1.85064939283218	3.65368823984073	0.52629853379699
C	0.84674602604160	4.61723127653900	0.73008474486521
H	2.90090335002662	3.95481963063227	0.52407012936891
C	-0.73852717699246	2.78791423466882	0.51211597974179
C	-0.47842062689809	4.14053619566074	0.71514585860881
H	-1.76155325045451	2.40359340695257	0.50176196293553
H	-1.32482817904116	4.81263587128760	0.86274765197702
C	0.00010135343780	0.00000197746832	3.20003390373280
C	-1.31433284941974	0.03779437526068	3.65259131879683
C	1.11528606075711	-0.00249521422326	4.02151548020559
C	-1.48980519414666	0.08522311379907	5.05500634736818
C	0.91516396176272	0.04391782872956	5.41441597089857
C	-0.39049799728877	0.08858006329859	5.92198974432542
H	-2.50640442263968	0.11557622838803	5.46679805343663
H	1.77455310960702	0.04205877207888	6.09397513531893
Cl	-1.16225736968858	-1.65850455117383	-0.69690215074242
N	1.92019555007335	0.00014800669005	-0.04909767111610
N	0.23270645519628	1.86579922442754	0.32588866953133
H	2.13066227881084	-0.04158284878602	3.61207668141166
H	-0.55406254822016	0.12313956340008	7.00361114507540
C	6.26610947621015	0.44520907344228	-0.21349446433827
C	1.21248483377730	6.09223126970839	0.95614596755111
C	6.62485056789746	1.41225395488430	-1.36934379443281
H	6.28463614660838	1.01706482721432	-2.33950454126054
H	6.17021335012357	2.40601111940014	-1.23428164899777
H	7.71687043242882	1.55195256190890	-1.42307807205858
C	6.75923946752600	1.04039669077344	1.12902300909438
H	6.30795625987289	2.02296998813491	1.33730951782996
H	6.51728086700749	0.37491184157561	1.97262663718014
H	7.85282703109415	1.17615436440093	1.10586524018003
C	6.99744067575181	-0.89039185632573	-0.45170131478998
H	6.80560345640667	-1.61688461171685	0.35408634685616
H	6.71204615358196	-1.35358444748502	-1.40976352478962
H	8.08449179287115	-0.71730548104867	-0.48355757118451
C	1.99036371941745	6.62145506345287	-0.27449400206859
H	2.92205693018622	6.06063477467824	-0.44777407544249
H	1.38231465859708	6.55217859930613	-1.19032752824313
H	2.26318314290944	7.67914750969811	-0.12653220889647
C	2.10294886225384	6.20821330104968	2.21857356602592
H	1.57838957610029	5.83393862791580	3.11160780908170
H	3.03965537391469	5.63809542846765	2.11785708793579
H	2.37352935837938	7.26163969075307	2.39794457782866
C	-0.03604340512877	6.97290961148726	1.15855770290728
H	-0.70119652277142	6.95629208034579	0.28023671409624
H	-0.62017392808342	6.66552034344488	2.04069533153758
H	0.26943382169612	8.01895158439566	1.31722509775604
C	-2.49294577945819	0.01874228463116	2.70536638134371
H	-3.16695198192637	0.87662249890543	2.86991704337478
H	-2.13561107907426	0.03808510445606	1.66566285611816
H	-3.09276903958773	-0.89897777287036	2.81979104355909



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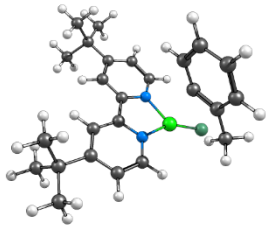
Aryl Chloride RKS 3.4 Å Ni–C distance

Ni	-0.00017893471236	-0.00024475468956	0.00184845822685
C	-2.46768238949029	1.18487287376308	0.02382010827172
C	-2.65362848133260	-1.14447987830255	-0.10259793602616
C	-3.85708329067306	1.31336093490541	0.00120687385777
C	-4.04395359659154	-1.05942332426018	-0.12736565427421
H	-2.12414169004662	-2.09813623140883	-0.13561777105958
C	-4.69527957969178	0.18663714149686	-0.07556696659771
H	-4.29154718516877	2.31482063513266	0.04333218184275
H	-4.60621204976288	-1.99225481273665	-0.18757908805867
C	-1.51178438113796	2.29756592468407	0.10296200217332
C	-1.83644060177921	3.65372585440080	0.18249456328996
C	-0.83427143508826	4.63839791703680	0.25340156443789
H	-2.88939528084649	3.94456631202044	0.19025535286218
C	0.76858528148268	2.80820174756257	0.15939349339368
C	0.49330550084797	4.17253661362427	0.23940678190161
H	1.78753702047606	2.41340380968675	0.14623265448510
H	1.33689622112073	4.86235524360892	0.29033777627737
C	-0.00006143329882	-3.40024421833917	-0.00006151783200
C	0.40674460627790	-3.86820090930321	-1.24748442830839
C	-0.32681874685589	-4.21530788804334	1.06931269398022
C	0.45276300556166	-5.27100734707226	-1.40703048353080
C	-0.27229686747656	-5.61395810146134	0.88795574562149
C	0.11612245498086	-6.13144116961559	-0.35217611547649
H	0.76539056226425	-5.69099407830659	-2.37127927574585
H	-0.52744915579569	-6.28436597657168	1.71642731852157
Cl	2.14357998093372	-0.14002450607777	0.00236911527190
N	-1.85093738601399	-0.04847970734164	-0.02769487474552
N	-0.20511757395055	1.87459832066649	0.09139375422250
H	-0.61465466803486	-3.80166929752528	2.04228664172232
H	0.16589982394616	-7.21472662520168	-0.50101251518929
C	-6.22264606360656	0.34739090155999	-0.09930025663764
C	-1.20753120891140	6.12616364261164	0.34062995433713
C	-6.62734941883466	1.19757876961902	-1.32952478762291
H	-6.31369330114667	0.71439012450617	-2.26825113862445
H	-6.17891487715429	2.20307564408617	-1.30397256284278
H	-7.72185414172585	1.32386094996293	-1.36117553393154
C	-6.68070180434105	1.06387171310933	1.19563849579081
H	-6.23384674738268	2.06543222326748	1.29515906887624
H	-6.40568465563897	0.48368308147348	2.09052046546740
H	-7.77584951205249	1.18853823275905	1.19439562099017
C	-6.94493876244450	-1.01123857773635	-0.18652820798264
H	-6.72038331265671	-1.65558891101490	0.67845608124846
H	-6.68215414171469	-1.56144278025828	-1.10415049522854
H	-8.03445023034234	-0.85195812663520	-0.20144742169778
C	-2.03000208826021	6.51959831222599	-0.91184703732476
H	-2.96194336636383	5.93888046445119	-0.99506129991410
H	-1.45130850007351	6.35905964312357	-1.83510558439659
H	-2.30687989065832	7.58540218577545	-0.86506536498180
C	-2.05866251322676	6.36464708554112	1.61288179221477
H	-1.50108312644308	6.09096839791254	2.52240774625939
H	-2.99178804500510	5.78004890606887	1.60305117913588
H	-2.33527783246375	7.42869674508986	1.69082109610184
C	0.03756767443613	7.03178935399035	0.41040142176399
H	0.67382820337529	6.93049915374148	-0.48330315090389
H	0.65378214361593	6.82058691291768	1.29889901616076
H	-0.27400725149862	8.08618067281464	0.47189119372878
C	0.79468929003166	-2.92387533139729	-2.36114303860808
H	1.65024808576644	-2.30134732926435	-2.05483923019328
H	-0.03001348426271	-2.22755470525807	-2.58887328484277
H	1.05958330583951	-3.46004582037538	-3.28592638485755



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Aryl Chloride Triplet 3.4 Å Ni–C distance

Ni	-0.00161283009671	0.00025304921980	0.00053141904558
C	2.50344283571986	1.21866697197054	0.23283101473594
C	2.71685666457783	-1.06592491282778	-0.19724837715637
C	3.89347261097800	1.36349884076922	0.24943383873479
C	4.10795613763922	-0.97814475064710	-0.18777360363351
H	2.19860601774561	-2.01197688427486	-0.37562028664708
C	4.74054758266294	0.25959132009392	0.03967879857634
H	4.32203147693278	2.35211896814621	0.43033990562977
H	4.68553833877428	-1.88718603988601	-0.36064371581610
C	1.51871012965708	2.29642694059733	0.43263311949357
C	1.82429616751005	3.64046231385493	0.65704786400484
C	0.81160949153777	4.60136457476008	0.82916401787602
H	2.87352002581641	3.94268820775987	0.69790495585345
C	-0.76136208851018	2.77293104917971	0.52717521957368
C	-0.51128038892267	4.12358437851287	0.75362753030722
H	-1.78251538216714	2.38764472506864	0.46950138920536
H	-1.36389264356038	4.79381147520775	0.87132792562629
C	0.00411121394320	-0.00313365107224	3.40052491603511
C	-1.33778159500931	0.05315909233220	3.75548569511074
C	1.06573633764862	-0.00511728290399	4.28768980775304
C	-1.60406002782482	0.12226842994923	5.14303513031831
C	0.77221306358332	0.06294713399495	5.66339302107386
C	-0.56426929136518	0.12735172078716	6.08073550633684
H	-2.64527382408491	0.16878690168370	5.48562672538058
H	1.58397160959830	0.06300590546029	6.39894854844395
Cl	-1.15999524583745	-1.66784428649163	-0.67339945150062
N	1.91695160612997	0.00056536713104	0.00839678750901
N	0.21797615799245	1.85209860230874	0.37403998842016
H	2.10464172040359	-0.05950497013217	3.94515416964547
H	-0.79930089954968	0.17928762842508	7.14830566978812
C	6.26742646609057	0.43403646881103	0.06281110499417
C	1.16578324779211	6.07432967887296	1.08475742680308
C	6.68302050040579	1.43885580860036	-1.04059496622766
H	6.38769541465674	1.07896989631927	-2.03879841442571
H	6.22514675613522	2.42926979837057	-0.89250525921899
H	7.77675091702716	1.57565141415810	-1.03814338116143
C	6.69803812050744	0.98069394331579	1.44680489281817
H	6.23849677627728	1.95657861284827	1.66803245947840
H	6.41609344735244	0.28680437265063	2.25435112148905
H	7.79168901870394	1.11415942769120	1.47956532294879
C	7.00605831917283	-0.89548082124186	-0.18660610954178
H	6.77427557471247	-1.64855394000580	0.58348675946120
H	6.76523303942623	-1.32414992724266	-1.17257846042517
H	8.09384776223273	-0.72592229902396	-0.16091257388687
C	1.99675419416083	6.61603210644994	-0.10507897199763
H	2.93619987334634	6.05807552233225	-0.24189100170834
H	1.43014309980256	6.55442747495942	-1.04764250366372
H	2.26102744954690	7.67266001880897	0.06457918889615
C	1.99953707015614	6.17882038934526	2.38627931619225
H	1.43611750398298	5.79639823844475	3.25178416225948
H	2.93974969260469	5.60922200006229	2.32168266077284
H	2.26182840303148	7.23049248009065	2.58721230264583
C	-0.09128454569994	6.95245352345441	1.23998481823834
H	-0.71719519572905	6.94292702993689	0.33317260498317
H	-0.71332462846095	6.63700291967064	2.09288898742557
H	0.20581682956930	7.99728923042556	1.42104983615452
C	-2.44787011453185	0.02876766185253	2.72963026720054
H	-3.14650089068659	0.87216828039370	2.86041858776194
H	-2.02118279752340	0.06935175345413	1.71683520121639
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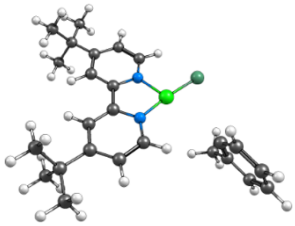

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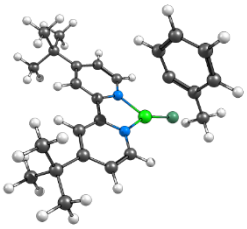
Aryl Chloride RKS 3.6 Å Ni–C distance

Ni	-0.00007248830926	-0.00018142256916	0.00123139967598
C	-2.50491137499401	1.10516674783016	0.01598504580161
C	-2.61422754968785	-1.23180571251961	-0.07612830171734
C	-3.89774101770213	1.18766810847804	-0.00544023671944
C	-4.00667448602127	-1.19248392258418	-0.09787146776416
H	-2.05204349543135	-2.16753285098600	-0.09400751147371
C	-4.69810405495508	0.03248277129606	-0.06443184598825
H	-4.36522076389975	2.17463084773266	0.02445002612474
H	-4.53835913655155	-2.14396234959101	-0.14100643893963
C	-1.58390889766433	2.24802395604488	0.08337256082652
C	-1.94906859656047	3.59463263837104	0.14599553769761
C	-0.97687785633307	4.60944391674036	0.21110502885323
H	-3.01029806256481	3.85387554402689	0.14509121347727
C	0.68081468784873	2.82752853958138	0.14483758193411
C	0.36423735028732	4.18364063302298	0.20914623128723
H	1.71134146050100	2.46418752455369	0.14033424231788
H	1.18637867076020	4.89907977658406	0.25721946060754
C	-0.00018837291810	-3.60018115340533	-0.00013098762629
C	0.38460130794399	-3.96310984283097	-1.28866376496688
C	-0.29948953603010	-4.49894169675816	1.00781714275392
C	0.44084865707157	-5.34880395861704	-1.55967104997101
C	-0.23599261629048	-5.87864907441252	0.71492956316276
C	0.13302416593943	-6.29263751176158	-0.56927575564974
H	0.73837799101170	-5.68868383497913	-2.55968468532085
H	-0.47045502068571	-6.61498280386157	1.49209257151858
Cl	2.14144904610402	-0.10655673314841	0.00182002557239
N	-1.84877854015043	-0.10784081767337	-0.02264821720568
N	-0.26480910698975	1.86513180149241	0.08252787910680
H	-0.57348979953190	-4.16791432092802	2.01624075115259
H	0.18980869174824	-7.36030741043176	-0.80382359361554
C	-6.23001262019064	0.14250098108680	-0.08826072306674
C	-1.39479361020958	6.08623364753011	0.28030272986509
C	-6.66360739581947	0.95927165965115	-1.33122097406269
H	-6.33522348553041	0.47169573016635	-2.26261133031127
H	-6.24838678113363	1.97922991551285	-1.32235255845185
H	-7.76169415790665	1.04902065042180	-1.36321109591024
C	-6.71031028882989	0.86384028597147	1.19586789591410
H	-6.29700727662080	1.88119337802514	1.27889239486027
H	-6.41533921290921	0.30734981275009	2.09940073539613
H	-7.80898767401609	0.95198110584802	1.19425410809932
C	-6.90714495410126	-1.24043716002419	-0.15300292744193
H	-6.66080754175492	-1.86321926254997	0.72178512375092
H	-6.62706638511990	-1.79621748251328	-1.06209424418163
H	-8.00132540231187	-1.11742508788436	-0.16903086937409
C	-2.22305440159664	6.44119852399281	-0.97983533794591
H	-3.13687216659759	5.83204803518881	-1.06055294135377
H	-1.63571854839061	6.28813052220833	-1.89889087891993
H	-2.53185693175977	7.49866772385850	-0.94582052157209
C	-2.25839217746163	6.31281032623617	1.54633434080302
H	-1.69699722997261	6.06582802628266	2.46113877334038
H	-3.17358057743772	5.70047354009552	1.53896724311000
H	-2.56701857439556	7.36887435333971	1.61144114125930
C	-0.17766764310001	7.02946095218625	0.34526987391236
H	0.46552134750588	6.93733280805569	-0.54445843335295
H	0.44038947664709	6.84688455456976	1.23882634250511
H	-0.52094867046421	8.07464275259868	0.39345698720368
C	0.73941597336894	-2.92894665323644	-2.33186529143704
H	1.59785659506803	-2.32463211689856	-1.99837181306035
H	-0.09546862465836	-2.22329782905784	-2.48134585904749
H	0.98414805875431	-3.38553351710880	-3.30374159344191



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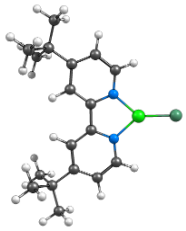
Aryl Chloride Triplet 3.6 Å Ni–C distance

Ni	0.00001768673953	-0.00001575769997	0.00006430360850
C	2.50388778285659	1.20667502804049	0.28752835596190
C	2.71716262083744	-1.06138389069967	-0.22372704700920
C	3.89370736928023	1.34449482563069	0.33746014870825
C	4.10814095879256	-0.97952367720141	-0.18618426004869
H	2.19876293860601	-1.99806161257817	-0.44613210675998
C	4.74072760272042	0.24575611790912	0.10138669121438
H	4.32200880118163	2.32315243169668	0.56700410642787
H	4.68581665187883	-1.88347425513342	-0.38382822581644
C	1.51835907350625	2.28005488956824	0.50371986112884
C	1.82080816554007	3.61935900233630	0.75766723952099
C	0.80598723206309	4.57651725795081	0.93883235906060
H	2.86956217822779	3.92130855280873	0.81234818848077
C	-0.76355661937018	2.75410412743964	0.58448886179169
C	-0.51605897897983	4.09988582537202	0.83957218508044
H	-1.78371800408436	2.36925147493148	0.50862182020257
H	-1.37008711332649	4.76758861427485	0.96158316605345
C	-0.00007937105396	0.00026316956645	3.60006428442219
C	-1.36147080642628	0.05630399012894	3.86485101000083
C	1.00931323929683	0.02579952124489	4.54418071389347
C	-1.70973771169216	0.15731628285259	5.23259144156188
C	0.63168127822319	0.12490955906530	5.89754715816597
C	-0.72819240983118	0.19110928554294	6.23062396580948
H	-2.76987172249311	0.20629194499051	5.51026517000617
H	1.39722908768625	0.14811063711419	6.68051851350028
Cl	-1.16158346072015	-1.67673540532504	-0.64289279826538
N	1.91689358046771	-0.00001624143615	0.00675846047789
N	0.21784837277303	1.83565957164096	0.42380238353292
H	2.06648503298911	-0.02994487169338	4.26410072715083
H	-1.02786455215465	0.26767173025109	7.28028695263460
C	6.26744839522669	0.41225350013574	0.16218662372092
C	1.15685218510453	6.04454503602685	1.22541222576264
C	6.70947322485315	1.45968303297919	-0.89009720934562
H	6.43351838053356	1.14237903995420	-1.90810075948306
H	6.25219257680102	2.44519389290782	-0.71082816530127
H	7.80341591696244	1.59147924399149	-0.85965841759588
C	6.67180113046612	0.89950377608190	1.57600857929103
H	6.21136493679982	1.86753569069703	1.82782595259829
H	6.37061968162486	0.17421884395503	2.34826249839823
H	7.76507021732652	1.02646133456757	1.63660817750000
C	7.00614803566049	-0.90918139703982	-0.12684743998565
H	6.75669504733337	-1.69194410770971	0.60727404231546
H	6.78298638786741	-1.29639489129400	-1.13391532815234
H	8.09384013059190	-0.74552281789167	-0.07318687304589
C	1.99056936890403	6.61120533792600	0.04915121678901
H	2.93059803035840	6.05645730975744	-0.09653238269810
H	1.42645784857832	6.56826683477514	-0.89594708788360
H	2.25368563866933	7.66439439454138	0.24087526168304
C	1.98640793481074	6.12520849805580	2.53127767761837
H	1.42129174612040	5.72431553839257	3.38728104460468
H	2.92829538255196	5.55940246752029	2.45826665978887
H	2.24564029611414	7.17328554936989	2.75387255890565
C	-0.10222549426171	6.91725872428035	1.39433499180456
H	-0.72404259834646	6.92717674635027	0.48472371047745
H	-0.72760297922039	6.58163305170114	2.23706089475412
H	0.19236330789369	7.95827288450305	1.59996722131141
C	-2.40660955258228	-0.00191594365600	2.77467386229897
H	-3.14164105083609	0.81462152237274	2.86858748281095
H	-1.92619739358251	0.05834147226499	1.78705557369468
H	-2.96244534585768	-0.95343024110644	2.79722317386600



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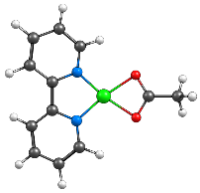
Aryl Chloride Putative Ni(I) Doublet—Phenyl Dissociated

Ni	1.12131625375462	-1.34044278348043	-0.10634848196161
C	-0.62447086581501	0.83102322737365	-0.03978139346347
C	1.60385834795871	1.52979173152413	-0.06904919896757
C	-1.05732624177199	2.15867845760945	-0.01089231366487
C	1.22461873705866	2.86929701629985	-0.04072508602992
H	2.65569241462020	1.23173859359291	-0.09290411452293
C	-0.13916778159110	3.22524151722763	-0.01038811277372
H	-2.13067376042035	2.36362671375235	0.01158757911198
H	2.00848615690703	3.62813389477213	-0.04268621505961
C	-1.48747078697437	-0.36158915120203	-0.04266927761879
C	-2.88392936937386	-0.36563657291487	-0.01553874376663
C	-3.61000752224278	-1.57119228123815	-0.02066986175762
H	-3.41426373550057	0.58970747260770	0.01026451406004
C	-1.45451993638831	-2.69649333050396	-0.08103189087745
C	-2.84547947321066	-2.75520675820389	-0.05471662476976
H	-0.84253252224459	-3.60232159276041	-0.10780721148562
H	-3.32128593824976	-3.73695749682439	-0.06112053391825
Cl	2.84902396775385	-2.59273926627553	-0.15646579160000
N	0.71400908166937	0.51001102229262	-0.06915199739677
N	-0.76402843686432	-1.53250318803838	-0.07567497621455
C	-0.63203620410991	4.68039948162554	0.02196402700901
C	-5.14633863473835	-1.55803858693969	0.00965773516279
C	-1.46888147197341	4.90906824775261	1.30545260907858
H	-0.86809422441763	4.72512429418277	2.21012183934518
H	-2.34897267495299	4.24863123952838	1.34818073690335
H	-1.83250471909284	5.94906374990897	1.34382088802858
C	-1.51443792393366	4.95000968280246	-1.22245331838395
H	-2.39588355770541	4.29079356649425	-1.25484130454513
H	-0.94674255504053	4.79585198036774	-2.15367068708334
H	-1.87862980694690	5.99048018361612	-1.21396580993006
C	0.53531621483313	5.68677339064346	0.01722584507316
H	1.15609893922674	5.59584772619511	-0.88851929478285
H	1.18817303454198	5.56701319117071	0.89668718239548
H	0.14000136563794	6.71440680030916	0.04093570156401
C	-5.62698575779308	-0.83830419410573	1.29450031730898
H	-5.27505704329918	0.20408534398353	1.34067093863975
H	-5.26555836854063	-1.35397686810619	2.19819210885678
H	-6.72857930512399	-0.81830769015551	1.33148800053130
C	-5.67640647377261	-0.80068838203950	-1.23347184326501
H	-5.35086013281287	-1.28904709250182	-2.16553147250125
H	-5.32589842582464	0.24280972170727	-1.26236114556226
H	-6.77859598588820	-0.78023171481700	-1.22681362251068
C	-5.73745560564246	-2.98142907749125	0.00008283309589
H	-5.42072248600976	-3.56675927917144	0.87820006334712
H	-5.45618808281846	-3.54012746023954	-0.90697506315787
H	-6.83718670287697	-2.92707648033080	0.02271246805954



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Aryl Acetate Putative Ni(I) Doublet—Phenyl Dissociated

C	4.645468000	0.110289000	-0.075652000
C	3.849233000	1.252747000	-0.027611000
C	4.025680000	-1.145098000	-0.249013000
C	2.642315000	-1.205602000	-0.367861000
N	1.857829000	-0.097579000	-0.363931000
C	2.457940000	1.139153000	-0.179298000
C	1.490717000	2.223492000	-0.159147000
N	0.193938000	1.767603000	0.026352000
C	1.761004000	3.592939000	-0.309458000
H	4.296736000	2.233824000	0.152477000
H	5.729646000	0.185916000	0.038662000
H	4.613314000	-2.064528000	-0.300636000
H	2.105038000	-2.149103000	-0.493656000
C	0.715969000	4.513455000	-0.262353000
H	2.786755000	3.926763000	-0.487354000
C	-0.601651000	4.039956000	-0.090424000
H	0.914550000	5.581968000	-0.375804000
C	-0.818274000	2.672279000	0.029301000
H	-1.448486000	4.728183000	-0.039836000
H	-1.816692000	2.245499000	0.155461000
Ni	-0.008850000	-0.087806000	-0.165343000
O	-0.521630000	-2.014106000	-0.254652000
C	-1.743467000	-1.640678000	-0.152586000
O	-1.984898000	-0.385218000	-0.064177000
C	-2.861432000	-2.648778000	-0.105392000
H	-2.558611000	-3.585903000	-0.590646000
H	-3.764363000	-2.244573000	-0.583078000
H	-3.109648000	-2.870474000	0.945508000